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L1 HAS NO ANSWERS
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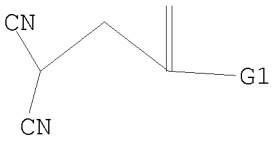


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G1 O,S


Structure attributes must be viewed using STN Express query preparation.


=> s l1 full
   REG1stRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.




FULL SEARCH INITIATED 15:53:36 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -     1160 TO ITERATE

100.0% PROCESSED     1160 ITERATIONS                              208 ANSWERS
SEARCH TIME: 00.00.01

L2          208 SEA SSS FUL L1



L3           78 L2

=> s l3 and py<2002
      21939583 PY<2002
L4           68 L3 AND PY<2002

=> s l4 and halo?
         407321 HALO?
L5            4 L4 AND HALO?

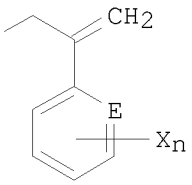
=> d 1-4 ibib abs hitstr

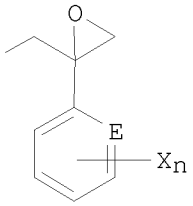
L5   ANSWER 1 OF 4  CAPLUS  COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER:         1998:76233  CAPLUS
DOCUMENT NUMBER:          128:177233
TITLE:                    Malononitrile derivatives and herbicides containing
                          them
INVENTOR(S):              Hosokawa, Akemi; Ikeda, Osamu
PATENT ASSIGNEE(S):       Mitsubishi Chemical Industries Ltd., Japan
SOURCE:                   Jpn. Kokai Tokkyo Koho, 18 pp.
                          CODEN: JKXXAF
```

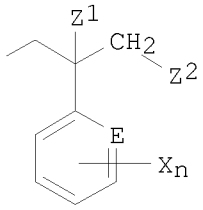
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 10029966	A	19980203	JP 1996-187796	19960717 <--

PRIORITY APPLN. INFO.: JP 1996-187796 19960717
OTHER SOURCE(S): MARPAT 128:177233
GI

Q = 

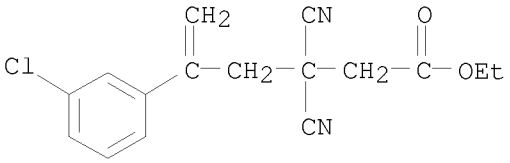
Q1 = 

Q2 = 

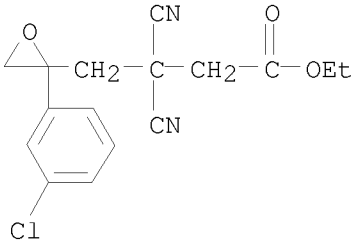
AB The derivs. are represented by R1R2C(CN)2 [I; R1 = H, C1-6 alkyl, C4-7 cycloalkyl, C2-6 alkenyl, C2-6 alkynyl, C1-6 haloalkyl, C2-6 haloalkenyl, C2-6 haloalkynyl, C2-8 alkoxyalkyl, C3-6 alkoxycarbonylalkyl, C2-4 cyanoalkyl, C1-6 hydroxyalkyl, C2-7 alkylamido, C7-9 aralkyl, C8-12 arylcarbonylalkyl, (un)substituted Ph, (un)substituted pyridyl, (un)substituted thiazolyl, CR3R4A; A = (un)substituted Ph, pyridyl, thiazolyl; R3-4 = H, Me; R2 = Q, Q1, Q2; E = CH, N; X = halo, C1-4 alkyl, C1-3 haloalkyl, NO2, C1-8 haloalkoxy, (un)substituted benzyloxy, pyridyloxy; n = 0-2; Z1-2 = OH, halo, C1-4 alkylsulfonyloxy, (un)substituted phenylsulfonyloxy]. The herbicides contain I as active ingredients. I (R1 = H, R2 = Q, E = CH, X = 3-Me, 5-Me) showed 91-100% herbicidal activity against Echinochloa oryzicola, Monochoria vaginalis, and Scirpus juncoides.

IT 203127-60-0P 203127-94-0P
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of malononitrile derivs. as herbicides)

RN 203127-60-0 CAPLUS
CN Benzenepentanoic acid, 3-chloro-β,β-dicyano-δ-methylene-, ethyl ester (CA INDEX NAME)



RN 203127-94-0 CAPLUS
CN Oxiranebutanoic acid, 2-(3-chlorophenyl)-β,β-dicyano-, ethyl ester (9CI) (CA INDEX NAME)

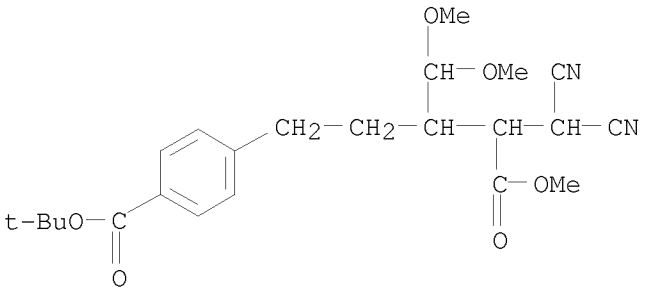


L5 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1993:213100 CAPLUS
DOCUMENT NUMBER: 118:213100
ORIGINAL REFERENCE NO.: 118:36739a,36742a
TITLE: Preparation of tricyclic fused pyrimidine compounds
INVENTOR(S): Akimoto, Hiroshi; Otsu, Koichiro; Miwa, Tetsuo
PATENT ASSIGNEE(S): Takeda Chemical Industries, Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 25 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 04211063	A	19920803	JP 1991-65613	19910305 <--
PRIORITY APPLN. INFO.:			JP 1990-54620 A1	19900305

OTHER SOURCE(S): MARPAT 118:213100
GI For diagram(s), see printed CA Issue.
AB The title compds. [I; Q1 = H, halo, radical linked through C, N, O, or S; one of Q2 and Q3 = N, the other = N, CH; Y = N, CR1 (wherein R1 = H, hydrocarbyl), methylidyne; Z = C2-5 bivalent radical containing optional substituents; ring A1, A2 = (substituted) 5-7-membered ring; B = (substituted) cyclic radical, etc.], useful as antitumor agents with high selectivity, are prepared Cyclocondensation of 1.181 g ester II (preparation given) with 314 mg guanidine HCl and Me3COK in Me3COH gave 1.02 g pyrrolopyrimidine III, which (1.010 g) was treated with borane-THF complex in THF at 0° and then at 50°, the solution cooled and stirred with HOAc-MeOH at room temperature to give 542 mg IV. The preferred doses of I are 2.0-500 mg/kg-day orally and 1.0-200 mg/kg injection.

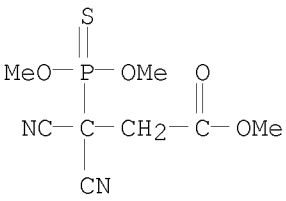
IT 147239-87-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, in preparation of antitumor agent)
RN 147239-87-0 CAPLUS
CN Benzenepentanoic acid, α-(dicyanomethyl)-β-(dimethoxymethyl)-4-[(1,1-dimethylethoxy)carbonyl]-, methyl ester (CA INDEX NAME)



L5 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1973:545978 CAPLUS
DOCUMENT NUMBER: 79:145978
ORIGINAL REFERENCE NO.: 79:23661a,23664a
TITLE: O,O-Dialkylthiophosphoric acid pseudochalcogen acyls
INVENTOR(S): Koehler, Helmut; Gerats, Irmtraut; Eichler, Gerhard; Kochmann, Werner
SOURCE: Ger. (East), 14 pp.
CODEN: GEXXA8
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DD 95374	A1	19730212	DD 1971-156303	19710705 <--

PRIORITY APPLN. INFO.: DD 1971-156303 A1 19710705
AB (MeO)2P(S)N(CN)CH2CO2R (I) and/or (MeO)2P(:NCN)SCH2CO2R (II) (R = Me or Et), prepared by reacting (MeO)2P(S)NNaCN with XCH2CO2R (X = Br or Cl), gave 95.0, 52.5 and 69.0% mortality for R = Me and 92.5, 51.0 and 55.0% for R = Et at 0.01, 1.0 and 0.05 weight % concentration, resp., against Musca domestica, Sitophylus granarius and Tetranychus urticae, resp. Analogs of I and II wherein the CO2R group was replaced by CONH2 and CONHMe, and (MeO)2P(S)C(CN)2CH2COR and (MeO)2P[: C(CN)2]SCH2COR (R = NHMe or OMe) were also prepared
IT 50605-40-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 50605-40-8 CAPLUS
CN Propanoic acid, 3,3-dicyano-3-(dimethoxyphosphinothioyl)-, methyl ester (CA INDEX NAME)



L5 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1964:484793 CAPLUS
DOCUMENT NUMBER: 61:84793
ORIGINAL REFERENCE NO.: 61:14826g-h,14827a-c
TITLE: 1-Halo-1,2,3,3-tetra(negatively substituted)propanes and their salts
INVENTOR(S): Martin, Elmore L.
PATENT ASSIGNEE(S): E. I. du Pont de Nemours & Co.
SOURCE: 6 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3133084		19640512	US	19600624 <--

PRIORITY APPLN. INFO.: US 19600624

AB Compds. of the general formula [XC(Z):C(Y)C(A)R]- M+ (I), where A, R, Y, Z are electron withdrawing groups such as CN, CO2Et, Bz, or SO2Ph, X is Cl or F, and M is H, Na, K, or a substituted ammonium ion, are dyes for natural and synthetic fibers. Thus, H2C(CN)2 79 in tetrahydrofuran (II) 220 was added with stirring to a dispersion 52 of 51.2% NaH in mineral oil and II 660 at 5-10° during 15 min., the mixture stirred 30 min., then dichlorofumaronitrile 44 in II 220 added during 15 min., II vaccum-distilled at 35-40°, the residual yellow solid dissolved in H2O 250, the pH adjusted to 8 with CO2, then Et4NBr 100 in H2O 200 parts added slowly with stirring, the mixture cooled to 5°, and the yellow crystals of I (A = R = Y = X = CN, Z = Cl, M = Et4N) (III) filtered, washed with 1% Et4NBr, and then H2O. The cake was dissolved in H2O 3500 at 100°, decolorizing carbon 10 added, the solution clarified, cooled to 5°, the long yellow needles filtered, washed with H2O and air-dried, giving 70 parts III, m. 129-31°, λmaximum 387 mμ, ε = 18,200 (MeOH) yellow on cellulose acetate and nylon, brownish yellow on wool and silk. Similarly, other I were prepared as tabulated below: X, Z, Y, A, R, M, % yield, m.p., color, λ (mμ)maximum, ε; Cl, PhN(CO-)2, CN, CN, Me4N, 31 230-5° (decompose), orange, 468, 12,200; Cl, CO2Me, CO2Me, CN, CN, Et4N, 82, 88-90°, yellow, 335, 29,400; Cl, CN, CN, CO2Et, CO2Et, H, 100, b1, 115-20°, yellow (Na salt), -, -; Cl, Bz, Bz, CN, CN, Me4N, 39, 210-12° (decompose), yellow, 416, 27,000; F, CF3, CF3, CN, CN, Pr4N, 81, 84-6°, yellow, -, -; Cl, CN, CN, CN, CN, Me4N, -, 217-18° (decompose), yellow, 386, 17,600; Cl, CN, CN, CN, CN, Pr4N, -, 74-6° (decompose), yellow, 386, 18,100; Cl, CN, CN, CN, CN, Et3NH, -, 63-5° (decompose), yellow, 387, 17,200; Cl, CN, CN, CN, CO2Et, Et4N, 56, 70-2°, yellow, 400, 15,700; Cl, CN, CN, CN,

SO2C6H4Me-4, Me4N, 73, 124-6° (decompose), yellow, 387, 17,000; Cl, CN, CN, CN, Bz, Me4N, -, 159-61°, yellow, 414, 17,100; Cl, CN, CN, CN, Bz, Et4N, 30 118-19°, yellow, 420, 16,200; Cl, CN, CN, CN, CN, Pr4N, -, 109-10°, yellow, 412, 17,600; Cl, CF3, CF3, CN, CN, Et4N, 64, 84-5°, yellow, -, -; F, -CF2CF2-, CN, CN, Na, -, -, orange, -, -; Cl, CN, CN, Bz, Bz, Me4n, -, 167°9°, yellow, 422, 8000; Cl, CN, CN, CN, CONHPh, K, -, -, red, -, -; Cl, CN, CN, SO2Ph, SO2Ph, Me4N, -, -, yellow, -, -; Cl, CN, CN, Bz, CO2Et, H, 20, 97-8°, colorless, -, -; Cl, CN, CN, Bz, CO,2Et, Na, yellow;

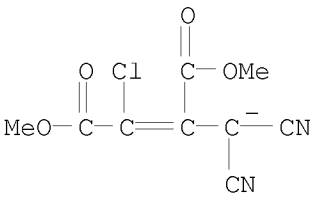
IT 98469-37-5P, Ammonium, tetraethyl, 1,2-dicarboxy-1-chloro-3,3-dicyanopropenide, dimethyl ester
RL: PREP (Preparation)
(preparation of)

RN 98469-37-5 CAPLUS

CN Tetraethylammonium 1,2-dicarboxy-1-chloro-3,3-dicyanopropenide, dimethyl ester (7CI) (CA INDEX NAME)

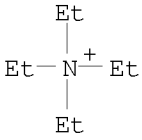
CM 1

CRN 98469-36-4
CMF C9 H6 Cl N2 O4



CM 2

CRN 66-40-0
CMF C8 H20 N



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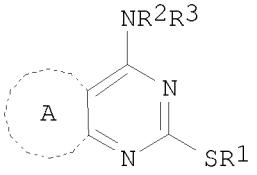
L4 ANSWER 1 OF 68 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2001:597989 CAPLUS
DOCUMENT NUMBER: 135:166840
TITLE: Preparation of pyrimidine compounds as modulators of chemokine receptor activity
INVENTOR(S): Bonnert, Roger; Cage, Peter; Hunt, Fraser; Walters,

Lain; Willis, Paul
PATENT ASSIGNEE(S): Astrazeneca Ab, Swed.
SOURCE: PCT Int. Appl., 52 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001058902	A1	20010816	WO 2001-SE245	20010207 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
GB 2359078	A	20010815	GB 2000-3019	20000211 <--
EP 1265899	A1	20021218	EP 2001-902950	20010207
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2003522189	T	20030722	JP 2001-558051	20010207
US 20030040523	A1	20030227	US 2002-203584	20020809
US 6958344	B2	20051025		
US 20050234077	A1	20051020	US 2005-36682	20050114

PRIORITY APPLN. INFO.:
GB 2000-3019 A 20000211
WO 2001-SE245 W 20010207
US 2002-203584 A1 20020809

OTHER SOURCE(S): MARPAT 135:166840
GI



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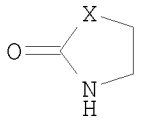

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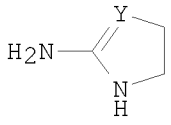
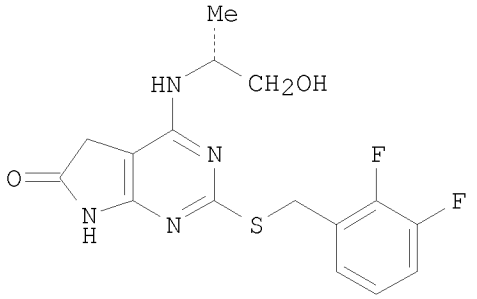


III



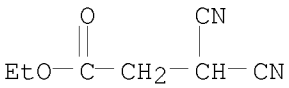
IV

AB The title compds. [I; A = II, III (X = NH, CR18R19; Y = N, CR18; R18, R19 = H, alkyl, Ph); R1 = (un)substituted cycloalkyl, alkyl, alkenyl, etc.; R2, R3 = H, cycloalkyl, alkyl, etc.; NR2R3 = (un)substituted 3-8 membered ring optionally containing one or more atoms selected from O, S, NH, etc.], useful in treating an inflammatory disease such as psoriasis and COPD, were prepared E.g., a multi-step synthesis of the 6H-pyrrolo[2,3-d]pyrimidin-6-one IV was given. The compds. I were found to have IC50 of < 10 μM against CXCR2 receptor binding.

IT 224637-77-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of pyrimidine compds. as modulators of chemokine receptor activity)

RN 224637-77-8 CAPLUS

CN Propanoic acid, 3,3-dicyano-, ethyl ester (CA INDEX NAME)



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 68 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2001:347933 CAPLUS

DOCUMENT NUMBER: 135:122094

TITLE: Cyclopropanation of benzylidenemalononitrile with dialkoxycarbenes and free radical rearrangement of the cyclopropanes

AUTHOR(S): Merkley, Nadine; Venneri, Paul C.; Warkentin, John

CORPORATE SOURCE: Department of Chemistry, McMaster University, Hamilton, ON, L8S 4M1, Can.

SOURCE: Canadian Journal of Chemistry (2001), 79(3), 312-318
CODEN: CJCHAG; ISSN: 0008-4042

PUBLISHER: National Research Council of Canada

DOCUMENT TYPE: Journal

LANGUAGE: English

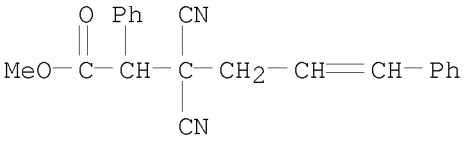
OTHER SOURCE(S): CASREACT 135:122094

AB Thermolysis of 2-cinnamyloxy-2-methoxy-5,5-dimethyl-Δ3-1,3,4-oxadiazoline (1a) and the analogous 2-benzyloxy-2-methoxy compound (1b) at 110°C, in benzene containing benzylidenemalononitrile, afforded products of apparent regiospecific addition of methoxycarbonyl and cinnamyl (or benzyl) radicals to the double bond. When the thermolysis of 1a was run with added TEMPO, methoxycarbonyl and cinnamyl radicals were captured. Thermolysis of the 2,2-dibenzyloxy analog (1c) in the presence of benzylidenemalononitrile gave an adduct that is formally the product of addition of benzyloxycarbonyl and benzyl radicals to the double bond. In this case, a radical addition mechanism could be ruled out, because the rate constant for decarboxylation of benzyloxycarbonyl radicals is very large. A mechanism that fits all of the results is predominant cyclopropanation of benzylidenemalononitrile by the dialkoxycarbenes derived from the oxadiazolines, in competition with fragmentation of the carbenes to radical pairs. The cyclopropanes so formed then undergo homolytic

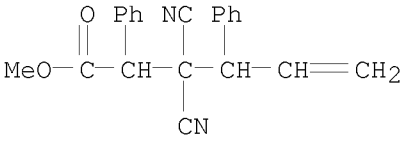
ring-opening to the appropriate diradicals. Subsequent β-scission of the diradicals to afford radical pairs, and coupling of those pairs, gives the final products. Thus, both carbene and radical chemical are involved in the overall processes.

IT 351207-62-0P 351207-63-1P 351207-65-3P
351207-66-4P 351207-67-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(cyclopropanation of benzylidenemalononitrile with dialkoxycarbenes and free radical rearrangement of the cyclopropanes)

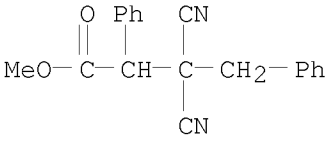
RN 351207-62-0 CAPLUS
CN Benzeneacetic acid, α-(1,1-dicyano-4-phenyl-3-butenyl)-, methyl ester (9CI) (CA INDEX NAME)



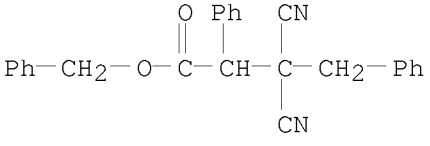
RN 351207-63-1 CAPLUS
CN Benzenebutanoic acid, β,β-dicyano-γ-ethenyl-α-phenyl-, methyl ester (CA INDEX NAME)



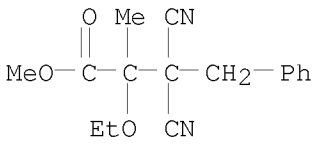
RN 351207-65-3 CAPLUS
CN Benzenebutanoic acid, β,β-dicyano-α-phenyl-, methyl ester (CA INDEX NAME)



RN 351207-66-4 CAPLUS
CN Benzenebutanoic acid, β,β-dicyano-α-phenyl-, phenylmethyl ester (CA INDEX NAME)

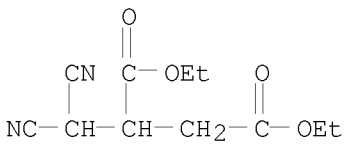


RN 351207-67-5 CAPLUS
CN Benzenebutanoic acid, β,β-dicyano-α-ethoxy-α-methyl-
, methyl ester (CA INDEX NAME)



REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 68 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2000:310730 CAPLUS
DOCUMENT NUMBER: 133:104844
TITLE: New aspects of knoevenagel condensation and michael addition reactions on alkaline carbonates
AUTHOR(S): Aramendia, Maria A.; Borau, Victoriano; Jimenez, Cesar; Marinas, Jose M.; Romero, Francisco J.
CORPORATE SOURCE: Department of Organic Chemistry, Faculty of Sciences, Cordoba University, Cordoba, E-14004, Spain
SOURCE: Chemistry Letters (2000), (5), 574-575
CODEN: CMLTAG; ISSN: 0366-7022
PUBLISHER: Chemical Society of Japan
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 133:104844
AB The Knoevenagel condensation of malononitrile with benzaldehyde on K2CO3, Rb2CO3 and Cs2CO3 gave the condensation product benzylidenemalononitrile but the reaction proceeded to the hydrogenated product benzylmalononitrile. Also, the Michael addition of malononitrile to certain double bonds occurs in the presence of K2CO3.
IT 82584-86-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(potassium carbonate catalyzed Michael addition reactions of malononitrile with alkenes)
RN 82584-86-9 CAPLUS
CN Butanedioic acid, (dicyanomethyl)-, diethyl ester (9CI) (CA INDEX NAME)



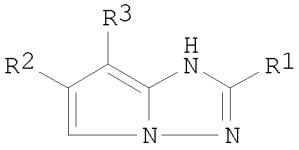
REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 68 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2000:199325 CAPLUS
DOCUMENT NUMBER: 132:237096

TITLE: Preparation of 1H-pyrrolo-[1,2-b][1,2,4]triazole
INVENTOR(S): Morita, Kensuke
PATENT ASSIGNEE(S): Fuji Photo Film Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 15 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2000086662	A	20000328	JP 1998-265064	19980918 <--

PRIORITY APPLN. INFO.: JP 1998-265064 19980918
OTHER SOURCE(S): CASREACT 132:237096; MARPAT 132:237096
GI



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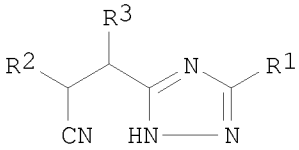
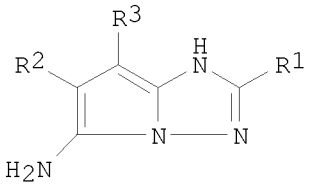


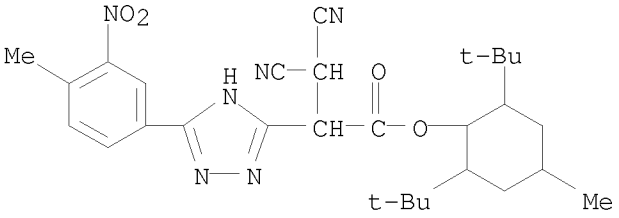
II



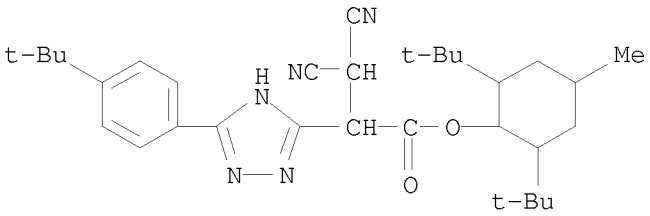
III

AB Title compds. I (R1-R3 = H, substituent) are prepared from triazoles II (R1-R3 = H, substituent) via III (R1- R3 = H, substituent). 3-(Tert-butylphenyl)-5-[[4-methyl-2,6-di-tert-butylhexyloxycarbonyl]bromomethyl]-1H-1,2,4-triazole was reacted with malononitrile in dimethylacetamide in the presence of NaOMe/MeOH under reflux for 30 min and reacted in the presence of CuCl in PhMe-hexane mixture under reflux for 3 h to give 91% III (R1 = 4-tert-butylphenyl; R2 = cyano, R3 = 4-methyl-2,6-di-tert-butylhexyloxycarbonyl), which was reacted with isoamyl nitrite in iso-Pr alc. at 50° for 10 h to give 40% I (R1-R3 = same as above).

IT 259266-71-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of pyrrolotriazoles from cyanoethyltriazoles)
RN 259266-71-2 CAPLUS
CN 1H-1,2,4-Triazole-3-acetic acid, α-(dicyanomethyl)-5-(4-methyl-3-nitrophenyl)-, 2,6-bis(1,1-dimethylethyl)-4-methylcyclohexyl ester (CA INDEX NAME)



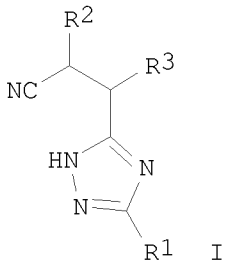
IT 259266-70-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of pyrrolotriazoles from cyanoethyltriazoles)
RN 259266-70-1 CAPLUS
CN 1H-1,2,4-Triazole-3-acetic acid, α-(dicyanomethyl)-5-[4-(1,1-dimethylethyl)phenyl]-, 2,6-bis(1,1-dimethylethyl)-4-methylcyclohexyl ester (CA INDEX NAME)



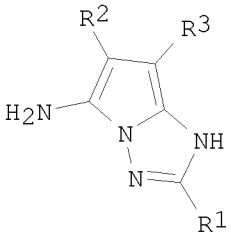
L4 ANSWER 5 OF 68 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2000:198039 CAPLUS
DOCUMENT NUMBER: 132:238369
TITLE: 1H-Pyrrolo[1,2-b][1,2,4]triazole derivatives and their manufacture
INVENTOR(S): Morita, Kensuke
PATENT ASSIGNEE(S): Fuji Photo Film Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 14 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2000086661	A	20000328	JP 1998-265059	19980918 <--

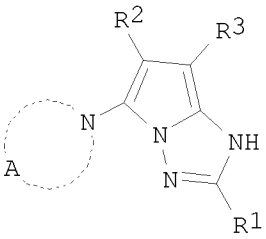
PRIORITY APPLN. INFO.: JP 1998-265059 19980918
OTHER SOURCE(S): MARPAT 132:238369
GI



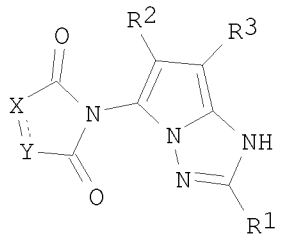
I



II



III



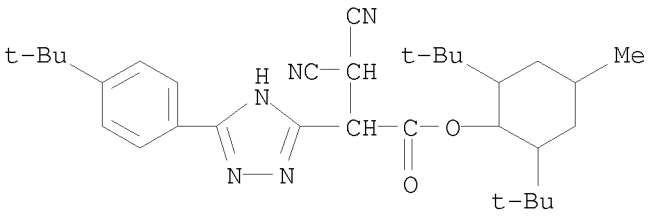
IV

AB The derivs. III and IV, useful for photog. couplers, physiol. active substances, etc., are manufactured from triazole derivs. I via intermediates II (R1-3 = H, substituent; A = non-metal atomic group to form azole ring with N; X, Y = non-metal atom to form 5-membered ring with CONCO). Thus, I (R1 = p-tert-BuC6H4; R2 = CN; R3 = 2,6-di-tert-butyl-4-methylcyclohexyloxycarbonyl) was treated with CuCl to give 91% II, 9.42 mmol of which was treated with 11.3 mmol acetonylacetone in benzene in the presence of AcOH to give 8.20 mmol III (azole ring = 3,4-dimethyl-1-pyrrolyl).

IT 259266-70-1P
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(manufacture of pyrrolotriazole derivs.)

RN 259266-70-1 CAPLUS

CN 1H-1,2,4-Triazole-3-acetic acid, α-(dicyanomethyl)-5-[4-(1,1-dimethylethyl)phenyl]-, 2,6-bis(1,1-dimethylethyl)-4-methylcyclohexyl ester (CA INDEX NAME)



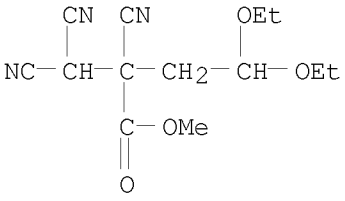
L4 ANSWER 6 OF 68 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2000:141061 CAPLUS
DOCUMENT NUMBER: 132:278722

TITLE: Spontaneous addition of active methine compounds to enol ethers and α,β-unsaturated ketones in aprotic polar solvent
AUTHOR(S): Yokozawa, Tsutomu; Oishi, Motoi; Tanaka, Yasukazu
CORPORATE SOURCE: Department of Applied Chemistry, Kanagawa University, Kanagawa-ku Yokohama, 221-8686, Japan
SOURCE: Journal of Organic Chemistry (2000), 65(6), 1895-1897
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 132:278722

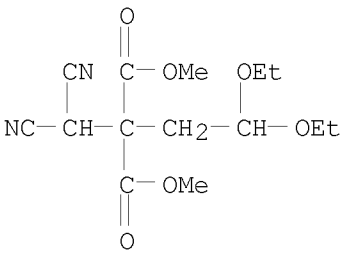
AB Addition of (EtO)2CHCH2CXYCH(CN)2 (I, X = Y = cyano; X = cyano, Y = CO2Me; X = Y = CO2Me) to enol ethers and α,β-unsatd. ketones in DMF at room temp is reported. Thus, reacting I (X = Y = cyano) with H2C:CHOEt gave (EtO)2CHCH2C(CN)2CH(OEt)Me in 63% yield. This reaction illustrates that the electron-withdrawing groups at the β-positions of the active methine group having the ones at the α and β positions were strongly affected on the acidity of I.

IT 184092-93-1 189348-52-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(addition of methine compds. to enol ethers and α,β-unsatd. ketones)

RN 184092-93-1 CAPLUS
CN Butanoic acid, 2-cyano-2-(dicyanomethyl)-4,4-diethoxy-, methyl ester (CA INDEX NAME)



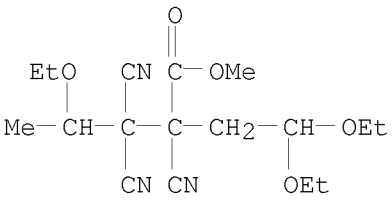
RN 189348-52-5 CAPLUS
CN Propanedioic acid, (dicyanomethyl)(2,2-diethoxyethyl)-, dimethyl ester (9CI) (CA INDEX NAME)



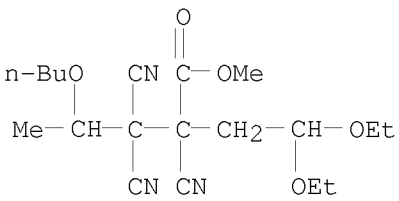
IT 264142-31-6P 264142-33-8P 264142-35-0P
264142-37-2P 264142-39-4P 264142-40-7P

264142-41-8P 264142-43-0P 264142-45-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(addition of methine compds. to enol ethers and α,β-unsatd. ketones)

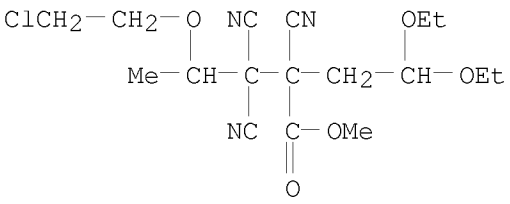
RN 264142-31-6 CAPLUS
CN Pentanoic acid, 2,3,3-tricyano-2-(2,2-diethoxyethyl)-4-ethoxy-, methyl ester (CA INDEX NAME)



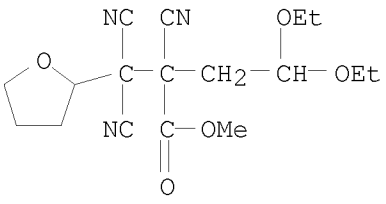
RN 264142-33-8 CAPLUS
CN Pentanoic acid, 4-butoxy-2,3,3-tricyano-2-(2,2-diethoxyethyl)-, methyl ester (CA INDEX NAME)



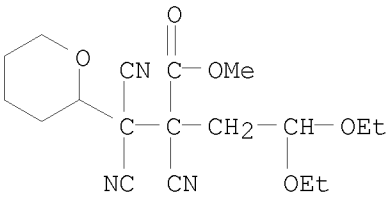
RN 264142-35-0 CAPLUS
CN Pentanoic acid, 4-(2-chloroethoxy)-2,3,3-tricyano-2-(2,2-diethoxyethyl)-, methyl ester (CA INDEX NAME)



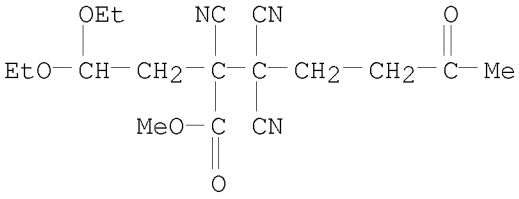
RN 264142-37-2 CAPLUS
CN 2-Furanpropanoic acid, α,β,β-tricyano-α-(2,2-diethoxyethyl)tetrahydro-, methyl ester (CA INDEX NAME)



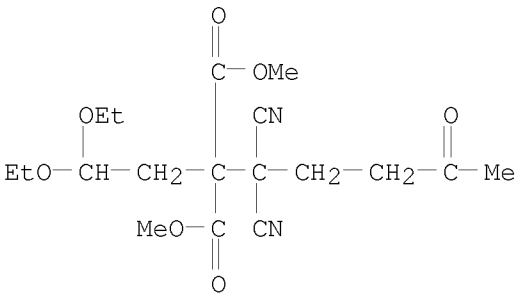
RN 264142-39-4 CAPLUS
CN 2H-Pyran-2-propanoic acid, α,β,β-tricyano-α-(2,2-diethoxyethyl)tetrahydro-, methyl ester (CA INDEX NAME)



RN 264142-40-7 CAPLUS
CN Heptanoic acid, 2,3,3-tricyano-2-(2,2-diethoxyethyl)-6-oxo-, methyl ester (CA INDEX NAME)

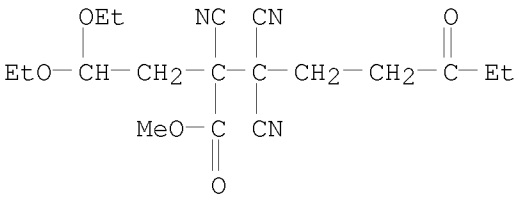


RN 264142-41-8 CAPLUS
CN Propanedioic acid, (1,1-dicyano-4-oxopentyl)(2,2-diethoxyethyl)-, dimethyl ester (9CI) (CA INDEX NAME)

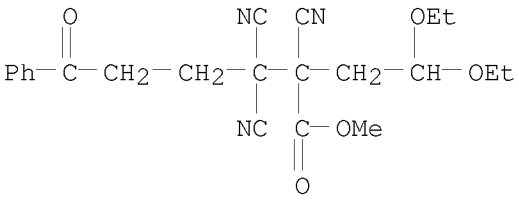


RN 264142-43-0 CAPLUS
CN Octanoic acid, 2,3,3-tricyano-2-(2,2-diethoxyethyl)-6-oxo-, methyl ester

(CA INDEX NAME)



RN 264142-45-2 CAPLUS
CN Benzenehexanoic acid, α,β,β-tricyano-α-(2,2-diethoxyethyl)-ε-oxo-, methyl ester (CA INDEX NAME)

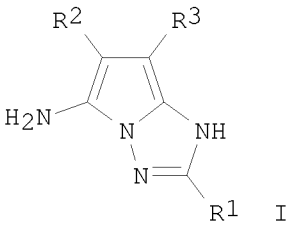


REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

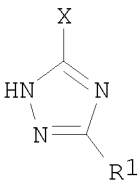
L4 ANSWER 7 OF 68 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2000:139178 CAPLUS
DOCUMENT NUMBER: 132:180579
TITLE: Preparation of 1H-pyrrolo[1,2-b][1,2,4]triazol-5-ylamines
INVENTOR(S): Morita, Kensuke
PATENT ASSIGNEE(S): Fuji Photo Film Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 15 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2000063382	A	20000229	JP 1998-232925	19980819 <--

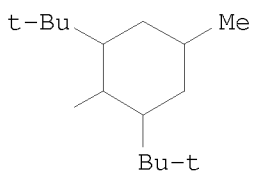
PRIORITY APPLN. INFO.: JP 1998-232925 19980819
OTHER SOURCE(S): CASREACT 132:180579; MARPAT 132:180579
GI



I



II

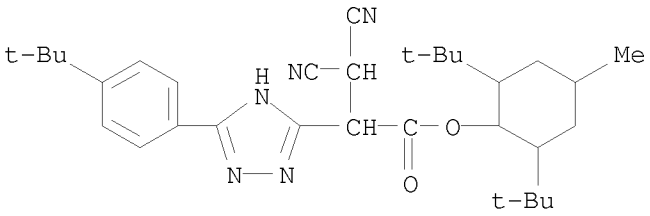
Q= 

AB Title compds. I (R1-R3 = H, substituent), useful as intermediates for physiol. active substances, photog. couplers, dyes, etc., are prepared from triazoles II (X = CHR3CHR2CN; R1-R3 = same as I). II (R1 = C6H4Bu-t-p, X = CHBrCO2Q) was treated with malononitrile and MeONa in DMF-MeOH under ice-cooling for 30 min and heated in the presence of CuCl in PhMe-hexane under reflux for 3 h to give 91% I (R1 = C6H4Bu-t-p, R2 = cyano, R3 = CO2Q).

IT 259266-70-1P 259266-71-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of pyrrolotriazolylamines as intermediates for physiol. active substances, dyes, and photog. couplers)

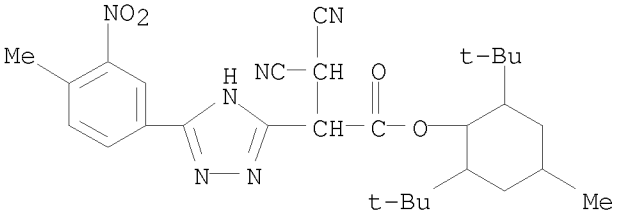
RN 259266-70-1 CAPLUS

CN 1H-1,2,4-Triazole-3-acetic acid, α-(dicyanomethyl)-5-[4-(1,1-dimethylethyl)phenyl]-, 2,6-bis(1,1-dimethylethyl)-4-methylcyclohexyl ester (CA INDEX NAME)

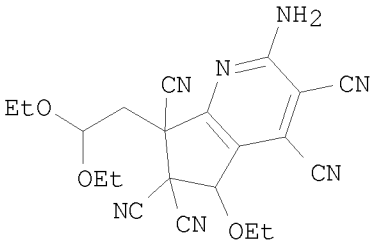


RN 259266-71-2 CAPLUS

CN 1H-1,2,4-Triazole-3-acetic acid, α-(dicyanomethyl)-5-(4-methyl-3-nitrophenyl)-, 2,6-bis(1,1-dimethylethyl)-4-methylcyclohexyl ester (CA INDEX NAME)



L4 ANSWER 8 OF 68 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1999:380253 CAPLUS
DOCUMENT NUMBER: 131:170252
TITLE: Tandem dimerization and double annulation of 3,3,4,4-tetracyanobutanal acetal. Synthesis of a bicyclic 2-aminopyridine derivative
AUTHOR(S): Yokozawa, Tsutomu; Nishikata, Akira; Kimura, Takamasa; Shimizu, Kazuki; Takehana, Tomoyuki
CORPORATE SOURCE: Department of Applied Chemistry, Kanagawa University, Yokohama, 221-8686, Japan
SOURCE: Tetrahedron Letters (1999), 40(25), 4707-4710
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 131:170252
GI

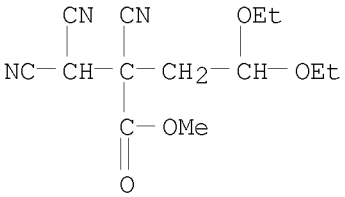


II

AB 3,3,4,4-Tetracyanobutanal acetal (I), which is easily obtained from tetracyanoethylene, Et vinyl ether, and ethanol, yielded 2-aminopyridine derivative II fused with cyclopentane in one pot in the presence of pyridine. On the basis of several expts., the proposed mechanism involves the Michael reaction of I with the diene generated by the elimination of hydrogen cyanide and ethanol from I, followed by double intramol. nucleophilic addns. to the cyano groups.

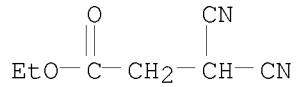
IT 184092-93-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of bicyclic aminopyridine by tandem dimerization-cyclization of tetracyanobutanal acetal)

RN 184092-93-1 CAPLUS
CN Butanoic acid, 2-cyano-2-(dicyanomethyl)-4,4-diethoxy-, methyl ester (CA INDEX NAME)



REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 9 OF 68 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1999:142792 CAPLUS
DOCUMENT NUMBER: 130:360507
TITLE: An N2S2 Bifunctional Chelator for Technetium-99m and Rhenium: Complexation, Conjugation, and Epimerization to a Single Isomer
AUTHOR(S): Luyt, Leonard G.; Jenkins, Hilary A.; Hunter, Duncan H.
CORPORATE SOURCE: Department of Chemistry, University of Western Ontario, London, ON, N6A 5B7, Can.
SOURCE: Bioconjugate Chemistry (1999), 10(3), 470-479
CODEN: BCCHES; ISSN: 1043-1802
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A bifunctional chelator HO2CCH(CH2NHCOCH2SH)2 6 (H3L) was prepared bearing an N2S2 core for binding Re or Tc and a carboxylic acid group for conjugation to amino groups of biomols. Complexation of 6 with Re(V) resulted in two kinetic isomers, anti-and syn-[ReO(HL)]- 7, being formed in approx. equal amts. Epimerization with 0.5M NaOH yields a single isomer anti-7, as determined by NMR spectroscopy and single-crystal x-ray anal. [99mTcO(HL)]- was prepared at the tracer level by reaction of the ligand with 99mTcO4-, SnCl2 and Na gluconate giving a mixture of two isomers, but showing a preference for the anti isomer. Chelation in the presence of 1 M NaOH results in anti-8 being formed as the sole product. The bifunctional ability of the ligand was explored by amide formation with (S)-α-phenethylamine, either by direct DCC coupling or through the RO2CCH(CH2NHCOCH2STr)2 9 (R = succinimidyl) intermediate. The deprotected bioconjugate PhCHMeNHOCCH(CH2NHCOCH2SH)2 11 (H2L1) was complexed with Re, yielding similar amts. of two isomeric Re complexes, anti- and syn-12, which were isolated and characterized by NMR spectroscopy. Treatment of the kinetic mixture of anti- and syn-[ReOL1]- 12 with 1 M NaOH resulted in quant. conversion to a single Re complex anti-12. With 99mTc in 0.1M NaOAc, bioconjugate 11 yielded anti- and sym-[99mTcOL1]- 13 in a 2:1 ratio, resp. In contrast, complexation in the presence of 1 M NaOH gave only one 99mTc complex, assigned the structure anti-13.
IT 224637-77-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reactant for preparation of rhenium and technetium bis(thioacetamidomethyl)propionate and bis(thioacetamidomethyl)propanamide complexes)
RN 224637-77-8 CAPLUS
CN Propanoic acid, 3,3-dicyano-, ethyl ester (CA INDEX NAME)



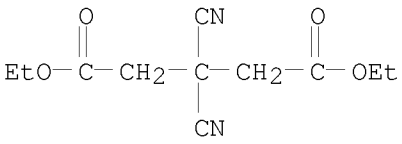
REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 10 OF 68 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1999:142376 CAPLUS
DOCUMENT NUMBER: 130:239567
TITLE: Diazaspirononanium salt for use as template for zeolite synthesis
INVENTOR(S): Kubota, Yoshihiro; Sugi, Yoshihiro
PATENT ASSIGNEE(S): Showa Denko K. K., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 9 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

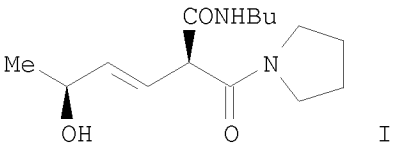
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 11060577	A	19990302	JP 1997-220414	19970815 <--

PRIORITY APPLN. INFO.: JP 1997-220414 19970815
OTHER SOURCE(S): MARPAT 130:239567
AB Claimed template is a salt of substituted 2,7-diazaspiro[4,4]nonanium. Hydrothermal synthesis of a zeolite by bringing a silica source and/or an alumina source into contact with the zeolite is also claimed. ZSM-12 zeolites having crystal size of a major axis ≥50 μm are also claimed.
IT 77415-69-1P
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(reaction of; diazaspirononanium salts as templates for manufacture of ZSM-12 zeolites having large crystal size)
RN 77415-69-1 CAPLUS
CN Pentanedioic acid, 3,3-dicyano-, diethyl ester (9CI) (CA INDEX NAME)



L4 ANSWER 11 OF 68 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1999:118566 CAPLUS
DOCUMENT NUMBER: 130:237421
TITLE: Stereoselective synthesis of alkenylated malonic diamide using masked acyl cyanide
AUTHOR(S): Nemoto, Hisao; Ibaragi, Touru; Bando, Masahiko; Kido, Masaru; Shibuya, Masayuki
CORPORATE SOURCE: Faculty of Pharmaceutical Sciences, the University of Tokushima, Tokushima, 770-8505, Japan
SOURCE: Tetrahedron Letters (1999), 40(7), 1319-1322
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal

LANGUAGE: English
OTHER SOURCE(S): CASREACT 130:237421
GI



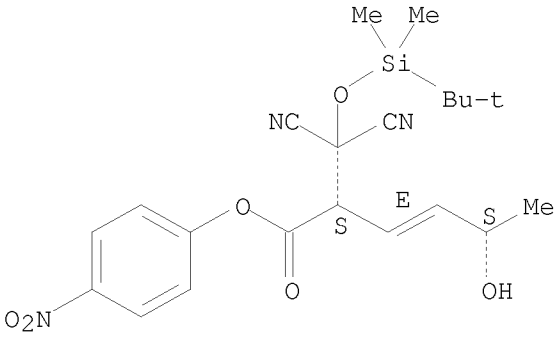
I

AB A highly stereoselective synthesis of an alkenylated malonic diamide (I) starting from a γ,δ-epoxy α,β-unsatd. carboxamide was accomplished using masked acyl cyanide (protected hydroxymalonitrile) via palladium-catalyzed regio- and stereoselective carbon-carbon bond formation.

IT 221219-72-3P 221219-73-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(stereoselective synthesis of alkenylated malonic diamide using masked acyl cyanide)

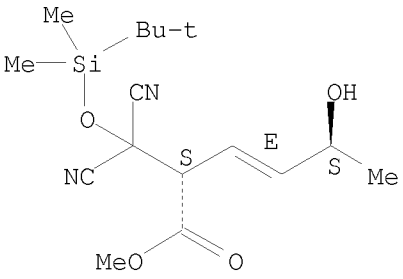
RN 221219-72-3 CAPLUS
CN 3-Hexenoic acid, 2-[dicyano[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-5-hydroxy-, 4-nitrophenyl ester, (2R,3E,5R)-rel- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



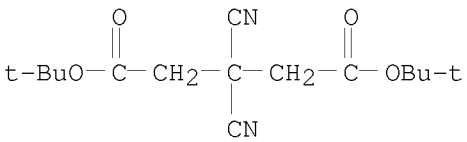
RN 221219-73-4 CAPLUS
CN 3-Hexenoic acid, 2-[dicyano[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-5-hydroxy-, methyl ester, (2R,3E,5R)-rel- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 12 OF 68 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1998:402031 CAPLUS
DOCUMENT NUMBER: 129:122635
TITLE: The reaction of phenacylmalononitrile with hydrazines: synthesis of new pyridazinones and pyrazolo[1,5-a]pyrimidines
AUTHOR(S): Elnagdi, Mohamed Hilmy; El-Ghamry, Ibrahim; Kandeel, Ezz; Abdel Rahman, A. H.; Al-Naggar, Abdul Aziz; Amer, Samir; Riad, Mohamed
CORPORATE SOURCE: Department of Chemistry, Faculty of Science, University of Kuwait, Safat, 13060, Kuwait
SOURCE: Gazzetta Chimica Italiana (1997), 127(12), 791-794
CODEN: GCITA9; ISSN: 0016-5603
PUBLISHER: Societa Chimica Italiana
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 129:122635
AB The reaction of phenacylmalononitrile with hydrazine hydrate affords a mixture of 3,5-diamino-4-phenacylpyrazole (I), and 6-oxo-3-phenyl-1,4,5,6-tetraydropyridazine-5-carbonitrile. The reaction of I with a variety of reagents, that enabled the synthesis of some new pyrazolo[1,5-a]pyrimidine derivs., is described.
IT 210347-41-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis of pyridazinones and pyrazolo[1,5-a]pyrimidines)
RN 210347-41-4 CAPLUS
CN Pentanedioic acid, 3,3-dicyano-, bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

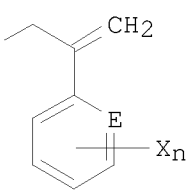


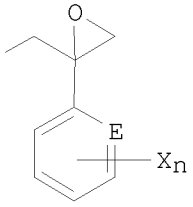
REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

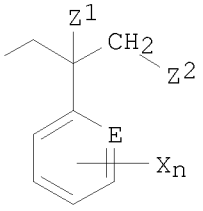
L4 ANSWER 13 OF 68 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1998:76233 CAPLUS
DOCUMENT NUMBER: 128:177233
TITLE: Malononitrile derivatives and herbicides containing them
INVENTOR(S): Hosokawa, Akemi; Ikeda, Osamu
PATENT ASSIGNEE(S): Mitsubishi Chemical Industries Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 18 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 10029966	A	19980203	JP 1996-187796	19960717 <--

PRIORITY APPLN. INFO.: JP 1996-187796 19960717
OTHER SOURCE(S): MARPAT 128:177233
GI

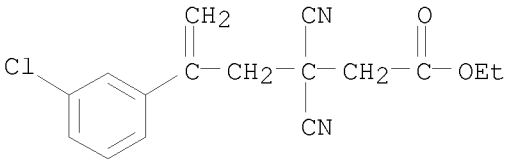
Q = 

Q1 = 

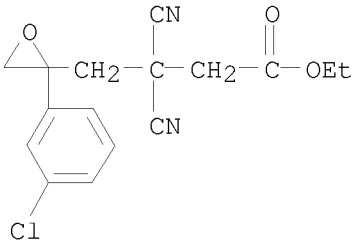
Q2 = 

AB The derivs. are represented by R1R2C(CN)2 [I; R1 = H, C1-6 alkyl, C4-7 cycloalkyl, C2-6 alkenyl, C2-6 alkynyl, C1-6 haloalkyl, C2-6 haloalkenyl, C2-6 haloalkynyl, C2-8 alkoxyalkyl, C3-6 alkoxycarbonylalkyl, C2-4 cyanoalkyl, C1-6 hydroxyalkyl, C2-7 alkylamido, C7-9 aralkyl, C8-12 arylcarbonylalkyl, (un)substituted Ph, (un)substituted pyridyl, (un)substituted thiazolyl, CR3R4A; A = (un)substituted Ph, pyridyl, thiazolyl; R3-4 = H, Me; R2 = Q, Q1, Q2; E = CH, N; X = halo, C1-4 alkyl, C1-3 haloalkyl, NO2, C1-8 haloalkoxy, (un)substituted benzyloxy, pyridyloxy; n = 0-2; Z1-2 = OH, halo, C1-4 alkylsulfonyloxy, (un)substituted phenylsulfonyloxy]. The herbicides contain I as active ingredients. I (R1 = H, R2 = Q, E = CH, X = 3-Me, 5-Me) showed 91-100% herbicidal activity against Echinochloa oryzicola, Monochoria vaginalis, and Scirpus juncoides.
IT 203127-60-0P 203127-94-0P
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic

preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of malononitrile derivs. as herbicides)
RN 203127-60-0 CAPLUS
CN Benzenepentanoic acid, 3-chloro-β,β-dicyano-δ-methylene-, ethyl ester (CA INDEX NAME)

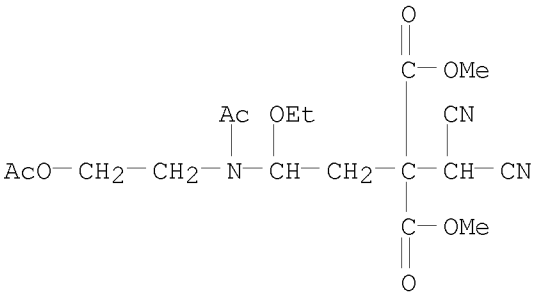


RN 203127-94-0 CAPLUS
CN Oxiranebutanoic acid, 2-(3-chlorophenyl)-β,β-dicyano-, ethyl ester (9CI) (CA INDEX NAME)



L4 ANSWER 14 OF 68 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1997:731010 CAPLUS
DOCUMENT NUMBER: 127:346753
TITLE: Synthesis of terpolymers by spontaneous copolymerization of the cyclobutane adducts of electron-acceptor olefins and vinyl ether with 2-oxazolines
AUTHOR(S): Yokozawa, Tsutomu; Tagami, Masato; Takehana, Tomoyuki; Suzuki, Tadashi
CORPORATE SOURCE: Dep. Appl. Chem., Kanagawa Univ., Yokohama, 221, Japan
SOURCE: Tetrahedron (1997), 53(45), 15603-15616
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Spontaneous copolymns. of the cyclobutane adducts of strong donors olefins and strong acceptor olefins, 1,1,2,2-tetracyano-3-ethoxycyclobutene (I) and di-Me 2,2-dicyano-3-ethoxycyclobutane-1,1-dicarboxylate (II), with 2-oxazolines are described. In the reaction of II with 2-methyloxazoline (III), the alternating copolymer of II and III, the 1:1:1 periodic terpolymer of di-Me 1,1-dicyanoethylene-2,2-dicarboxylate, vinyl ether, and III, was obtained. Cyclobutane I also reacted with III to yield copolymer rich in I.
IT 198274-09-8P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and characterization of)
RN 198274-09-8 CAPLUS
CN Propanedioic acid, [2-[acetyl[2-(acetyloxy)ethyl]amino]-2-ethoxyethyl](dicyanomethyl)-, dimethyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 15 OF 68 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1997:513581 CAPLUS
DOCUMENT NUMBER: 127:184884
TITLE: Multinuclear cluster complexes as diagnostic imaging contrast agents
INVENTOR(S): Droege, Michael; Yu, Shi-Bao; Sanderson, William; Bacon, Edward; Delecki, Daniel; Earley, William; Ye, Naidong
PATENT ASSIGNEE(S): Nycomed Salutar, Inc., USA
SOURCE: PCT Int. Appl., 51 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9726921	A2	19970731	WO 1997-GB211	19970123 <--
WO 9726921	A3	19971023		
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
CA 2241190	A1	19970731	CA 1997-2241190	19970123 <--
AU 9714523	A	19970820	AU 1997-14523	19970123 <--
EP 876161	A2	19981111	EP 1997-901180	19970123 <--
EP 876161	B1	20011121		
R: DE, DK, ES, FR, GB, IT, SE, IE, FI				
CN 1208353	A	19990217	CN 1997-191757	19970123 <--
HU 9901488	A2	19990830	HU 1999-1488	19970123 <--

BR 9707300	A	19991228	BR 1997-7300		19970123 <--
JP 2000515850	T	20001128	JP 1997-526668		19970123 <--
NO 9803371	A	19980722	NO 1998-3371		19980722 <--
PRIORITY APPLN. INFO.:			GB 1996-1340	A	19960123
			WO 1997-GB211	W	19970123

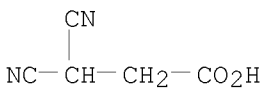
OTHER SOURCE(S): MARPAT 127:184884

AB Diagnostic imaging contrast media are claimed comprising a physiol. tolerable image contrast-enhancing complex, said complex comprising a pair of interconjugated multinuclear clusters, together with at least one pharmaceutical carrier or excipient. Included, for example, are multinuclear cluster complexes (M3)2L3 containing three metal atoms and L is a ligand. Clusters (M3)2L3 include M3 = M3SaOb where a = 1-4, b = 0-3 and a + b = 4, e.g., M3 = W3SO3. Ligands L include various polyaminocarboxylates and derivs. represented by general formula (R2)2N[(CHR4)mNR1]n(CHR4)mN(R2)2, e.g., N'-serinol-, N'-methyl-, and N'-benzyl-N,N,N'',N''-diethylenetriaminetetraacetic acids, various N'-(polyhydroxyalkyl)-N'-methyldiethylenetriaminetetraacetic acids, 2-carboxymethylpropylenediaminetetraacetic acid, etc., for which prepns. are given of these and other example ligands. Preparation of cluster compds., e.g., Na4[(W3SO3)2(EGTA)3] (EGTA = ethyleneglycol bis(2-aminoethyl ether)-N,N,N',N'-tetraacetate), from [W3SO3(H2O)9]Cl4 and the appropriate polyaminocarboxylic acid ligand, are described. The claimed preparation of [W3SO3(H2O)9]Cl4 comprises reaction of W(CO)6 and Na2S, followed by acidification of the product with at least 6 N HCl, and purification A charged contrast medium complex may be post-complexed with, e.g., cholamine hydrochloride or N-methyl-N,N-bis(hydroxyethyl)ethylenediamine, to give a preferred neutral derivative Pharmaceutically acceptable forms of the diagnostic imaging contrast media comprising said cluster complexes and dosages for the x-ray contrast media are briefly discussed.

IT 194083-97-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(for preparation of multinuclear tungsten aminocarboxylate cluster complexes as diagnostic imaging contrast agents)

RN 194083-97-1 CAPLUS

CN Propanoic acid, 3,3-dicyano- (CA INDEX NAME)



L4 ANSWER 16 OF 68 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1997:414890 CAPLUS
DOCUMENT NUMBER: 127:144690
TITLE: Metabolism and disposition of the antifolate LY231514 in mice and dogs
AUTHOR(S): Woodland, J. M.; Barnett, C. J.; Dorman, D. E.; Gruber, J. M.; Shih, C.; Spangle, L. A.; Wilson, T. M.; Ehlhardt, W. J.
CORPORATE SOURCE: Lilly Res. Laboratories, USA
SOURCE: Drug Metabolism and Disposition (1997), 25(6), 693-700
CODEN: DMDSAI; ISSN: 0090-9556

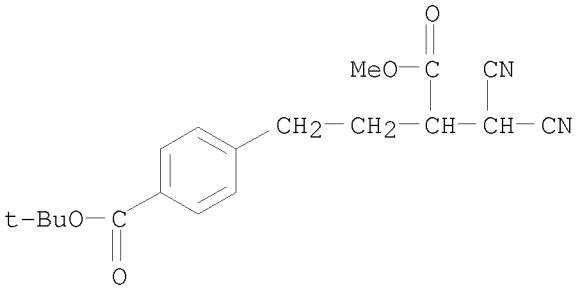
PUBLISHER: Williams & Wilkins
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The metabolism and disposition of LY231514 was studied in mice and dogs. LY231514 is a novel pyrrolopyrimidine-based multi-target antifolate (MTA) showing broad in vivo antitumor activity in mouse models and is currently in phase II human clin. trials. Doses (i.v.) of the compound showed high plasma levels, resulting in AUC values of 30-33 μg-hr/mL for mice and dogs after 20 and 7.5 mg/kg doses, resp. The compound was eliminated rapidly. Half-life values for mice and dogs were about 7 and 2 h, resp. In vitro plasma binding measured 56% in mice, 46% in dogs, and 81% in humans. Fecal elimination was the major excretion pathway in mice after single i.v. doses of [14C]LY231514. Urine constituted the major route of excretion in dogs. Parent LY231514 accounted for the majority of urinary radiocarbon in mice (90%) and dogs (68%). Minor metabolites were found in urine, but the amts. were too small to isolate or identify. Based on an earlier observation that LY231514 photodegraded to produce reaction products having similar retention times as these minor urinary isolates, a photo oxidation system was developed which in fact produced these metabolites. Subsequently, these photolytically produced materials were used as stds. to identity two novel in vivo metabolites formed by oxidation of the pyrrolo-pyrimidine ring system of LY231514. The oxidative transformations are similar to those observed for tryptophan and other indoles in that the pyrrole ring is oxidized to give an amide; further oxidation cleaves this ring, one ring carbon is lost, and a ketone is formed.

IT 193265-49-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(antifolate drug LY231514 metabolism and pharmacokinetics in mice and dogs)

RN 193265-49-5 CAPLUS

CN Benzenebutanoic acid, α-(dicyanomethyl)-4-[(1,1-dimethylethoxy)carbonyl]-, methyl ester (CA INDEX NAME)



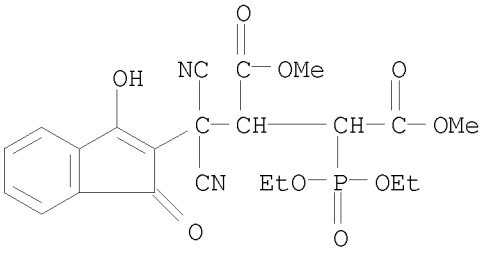
L4 ANSWER 17 OF 68 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1997:330734 CAPLUS
DOCUMENT NUMBER: 127:34293
TITLE: The reactions of Wittig-Horner reagents with 1,3-dioxo-Δ2,α-indanmalononitrile
AUTHOR(S): Boulos, Leila Sadek; Yakout, El-Sayed M. A.
CORPORATE SOURCE: National Research Centre, Cairo, Egypt
SOURCE: Heteroatom Chemistry (1997), 8(3), 253-257
CODEN: HETCE8; ISSN: 1042-7163

PUBLISHER: Wiley
DOCUMENT TYPE: Journal
LANGUAGE: English

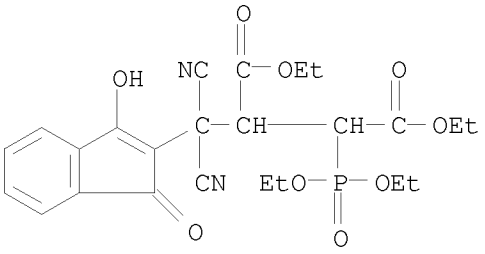
AB Wittig-Horner reagents react with 1,3-dioxo-Δ2,α-indanmalononitrile to give phosphonate adducts. Structural reasoning for the new products was based on compatible anal. and spectral data (IR, 1H, 31P NMR, and MS). The mechanism that accounts for the formation of the new adducts is discussed.

IT 190722-21-5P 190722-23-7P 190722-25-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

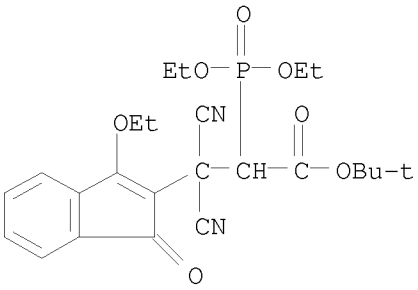
RN 190722-21-5 CAPLUS
CN Butanedioic acid, 2-[dicyano(3-hydroxy-1-oxo-1H-inden-2-yl)methyl]-3-(diethoxyphosphinyl)-, dimethyl ester (9CI) (CA INDEX NAME)



RN 190722-23-7 CAPLUS
CN Butanedioic acid, 2-[dicyano(3-hydroxy-1-oxo-1H-inden-2-yl)methyl]-3-(diethoxyphosphinyl)-, diethyl ester (9CI) (CA INDEX NAME)

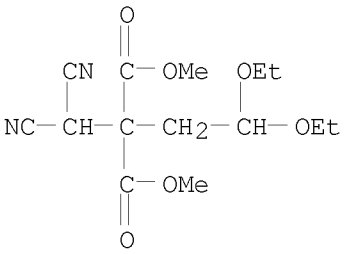


RN 190722-25-9 CAPLUS
CN 1H-Indene-2-propanoic acid, β,β-dicyano-α-(diethoxyphosphinyl)-3-ethoxy-1-oxo-, 1,1-dimethylethyl ester (CA INDEX NAME)

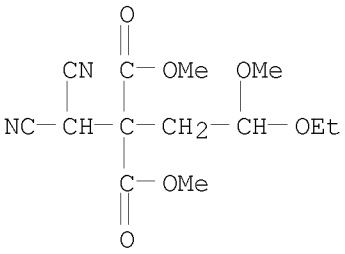


REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

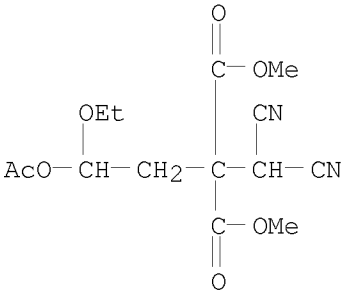
L4 ANSWER 18 OF 68 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1997:274825 CAPLUS
DOCUMENT NUMBER: 126:317775
TITLE: Ring-opening polymerization of cyclobutane adduct of dimethyl 1,1-dicyanoethylene-2,2-dicarboxylate and ethyl vinyl ether
AUTHOR(S): Yokozawa, Tsutomu; Wakabayashi, Yuki; Kimura, Takamasa
CORPORATE SOURCE: Dep. Applied Chem., Kanagawa Univ., Yokohama, 221, Japan
SOURCE: Journal of Polymer Science, Part A: Polymer Chemistry (1997), 35(8), 1563-1570
CODEN: JPACEC; ISSN: 0887-624X
PUBLISHER: Wiley
DOCUMENT TYPE: Journal
LANGUAGE: English
AB For an extension of the work on the ring-opening polymns. of cyclobutane adducts of strong donor olefins and strong acceptor olefins yielding novel alternating copolymers of those olefins, the ring-opening polymerization of the cyclobutane adduct (I; di-Me 2,2-dicyano-3-ethoxy-1,1-cyclobutanedicarboxylate) of di-Me 1,1-dicyanoethylene-2,2-dicarboxylate (DDED) and Et vinyl ether (EVE) is investigated. I reacted with methanol and acetic acid at ambient temperature to yield the corresponding ring-opened adducts. Polymns. of I were carried out with anionic initiators, tertiary amines, ammonium halides, and Lewis acids, resp., according to the polymerization methods of the cyclobutane adduct of tetracyanoethylene and EVE. All these polymerization catalysts except for ammonium halides were effective for the polymerization of I, yielding alternating copolymers of DDED and EVE. The chain transfer reactions of the polymerization with anionic initiators are also discussed on the basis of a model reaction.
IT 189348-52-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(model reaction for determination of mechanism; ring-opening polymerization of di-Me 2,2-dicyano-3-ethoxy-1,1-cyclobutanedicarboxylate)
RN 189348-52-5 CAPLUS
CN Propanedioic acid, (dicyanomethyl)(2,2-diethoxyethyl)-, dimethyl ester (9CI) (CA INDEX NAME)



IT 189348-50-3P 189348-51-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(model reactions for polymerization; reactions of di-Me 2,2-dicyano-3-ethoxy-
1,1-cyclobutanedicarboxylate with acetic acid and methanol)
RN 189348-50-3 CAPLUS
CN Propanedioic acid, (dicyanomethyl)(2-ethoxy-2-methoxyethyl)-, dimethyl ester (9CI) (CA INDEX NAME)

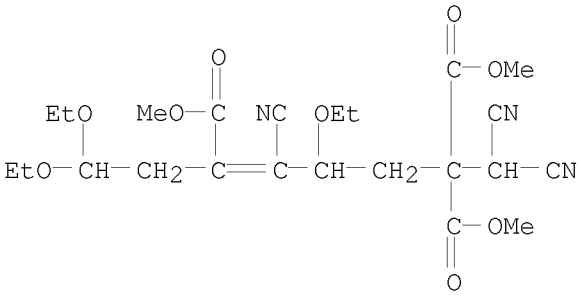


RN 189348-51-4 CAPLUS
CN Propanedioic acid, [2-(acetyloxy)-2-ethoxyethyl](dicyanomethyl)-, dimethyl ester (9CI) (CA INDEX NAME)



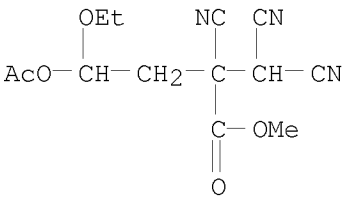
IT 189348-53-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(ring-opening polymerization of di-Me 2,2-dicyano-3-ethoxy-1,1-cyclobutanedicarboxylate)
RN 189348-53-6 CAPLUS
CN 5-Octene-2,2,6-tricarboxylic acid, 1,1,5-tricyano-4,8,8-triethoxy-,

trimethyl ester (9CI) (CA INDEX NAME)

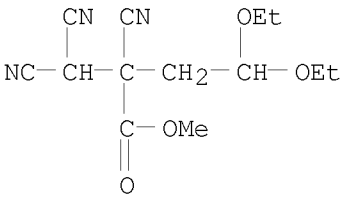


REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 19 OF 68 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1996:672685 CAPLUS
DOCUMENT NUMBER: 126:8777
TITLE: Ring-Opening Polymerization of the Cyclobutane Adduct of Methyl Tricyanoethylenecarboxylate and Ethyl Vinyl Ether
AUTHOR(S): Yokozawa, Tsutomu; Tsuruta, Ei-ichi
CORPORATE SOURCE: Department of Applied Chemistry, Kanagawa University, Yokohama, 221, Japan
SOURCE: Macromolecules (1996), 29(25), 8053-8056
CODEN: MAMOBX; ISSN: 0024-9297
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The ring-opening polymns. of a cyclobutane adduct (I) of Me tricyanoethylenecarboxylate (MTCE) and Et vinyl ether (EVE) are investigated. The adduct I reacted with acetic acid and ethanol at ambient temperature to yield the ring-opened corresponding adducts in good yields. I was polymerized with Lewis acids, anionic initiators, tertiary amines, and ammonium halides. All the catalysts except for ammonium halides were effective for the alternating polymerization similar to the polymerization of cyclobutane adduct of TCNE and EVE.
IT 184092-92-0P 184092-93-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(ring-opening reactivity of cyclobutane adduct of Me tricyanoethylenecarboxylate with ethanol or acetic acid and Et vinyl ether)
RN 184092-92-0 CAPLUS
CN Butanoic acid, 4-(acetyloxy)-2-cyano-2-(dicyanomethyl)-4-ethoxy-, methyl ester (CA INDEX NAME)



RN 184092-93-1 CAPLUS
CN Butanoic acid, 2-cyano-2-(dicyanomethyl)-4,4-diethoxy-, methyl ester (CA INDEX NAME)



REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 20 OF 68 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1996:664756 CAPLUS
DOCUMENT NUMBER: 125:329472
TITLE: Preparation of ring-fused pyrimidine-containing amino acid derivatives as antiprotozoan agents
INVENTOR(S): Horii, Toshihiro; Aono, Tetsuya
PATENT ASSIGNEE(S): Takeda Chemical Industries Ltd, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 31 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
JP 08225574	A	19960903	JP 1995-330939		19951220 <--
PRIORITY APPLN. INFO.:			JP 1995-330939	A	19951220
			JP 1994-317938		19941221

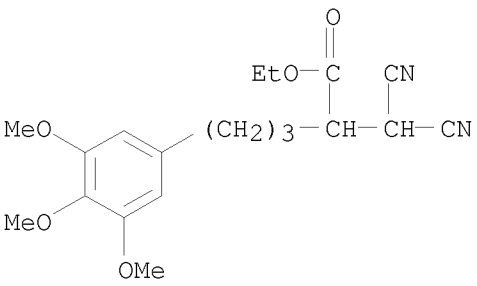
OTHER SOURCE(S): MARPAT 125:329472
GI For diagram(s), see printed CA Issue.
AB The title compds. [I; ring A = (un)substituted five membered ring; Z = (un)substituted bivalent aliphatic chain consisting of a series of <5 atoms and optionally interrupted by one hetero atom in the chain; B = (un)substituted 5- or 6-membered heterocyclyl or carbocyclyl; the substituent of B is preferably CONHCH(CO2R3)(CH2)pWR4; wherein p = 1-4; W = bond, O, NHCONH, NR, NRCO, CONR, NHSO2; wherein R = H, C1-4 hydrocarbyl; CO2R3 = optionally esterified CO2H; R4 = (un)substituted chain or cyclic group; or Z = (CR1R2)n-Z1; wherein R1, R2 = H,lower alkyl; Z1 = bond, O, NH; n = 1-5] or salts thereof, which are useful for treating infections of

protozoa, particularly coccidium and drug-resistant malaria, are prepared Thus, 4-[2-(2,4-diamino-7H-pyrrolo[2,3-d]pyrimidin-5-yl)ethyl]benzoic acid ditrifluoroacetate was condensed with Me O-(4-methoxycarbonylbenzyl)-L-serinate hydrochloride using di-Et cyanophosphate and Et3N in DMF at room temperature for 1 h to give 66% Me N-[4-[2-(2,4-diamino-7H-pyrrolo[2,3-d]pyrimidin-5-yl)ethyl]benzoyl]-O-O-(4-methoxycarbonylbenzyl)-L-serinate, which was saponified with a mixture of 1 h aqueous NaOH and MeOH at room temperature for 5 h and neutralized with dilute HCl to give 84% N-[4-[2-(2,4-diamino-7H-pyrrolo[2,3-d]pyrimidin-5-yl)ethyl]benzoyl]-O-O-(4-methoxycarbonylbenzyl)-L-serine. These compds. I inhibited dihydrofolic acid reductase of malaria protozoa Plasmodium falciparum with IC50 of 0.8-62 nM. The title compound (II; R5 = Q) showed ED50 of 0.17 and 0.11 nM for inhibiting the proliferation of wild type-malaria protozoa P. falciparum 3D7 and cycloguanyl-resistant P. falciparum FCR3, resp. Capsule, tablet, and vial formulations containing II (R5 = Q1) were prepared

IT 182961-44-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of ring-fused pyrimidine-containing amino acid derivs. as antiprotozoan agents)

RN 182961-44-0 CAPLUS

CN Benzenepentanoic acid, α-(dicyanomethyl)-3,4,5-trimethoxy-, ethyl ester (CA INDEX NAME)



L4 ANSWER 21 OF 68 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1996:365832 CAPLUS
DOCUMENT NUMBER: 125:86845
TITLE: Cyclopropenation and Related Reactions of Ruthenium Vinylidene Complexes
AUTHOR(S): Ting, Pei-Chen; Lin, Ying-Chih; Lee, Gene-Hsiang; Cheng, Ming-Chu; Wang, Yu
CORPORATE SOURCE: Department of Chemistry, National Taiwan University, Taipei, 106, Taiwan
SOURCE: Journal of the American Chemical Society (1996), 118(27), 6433-6444
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Facile deprotonation of a number of cationic ruthenium vinylidene complexes, followed by cyclopropenation, is accomplished in acetone. The

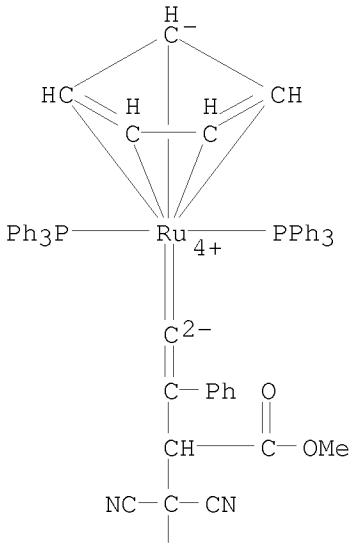
deprotonation of [Ru]:C:(Ph)CH2R+, ([Ru] = (η5-C5H5)(PPh3)2Ru through out this abstract) by n-Bu4NOH induces a novel cyclization reaction and yields the neutral cyclopropenyl complexes [cyclic] [Ru]-C:C(Ph)CHR (3b, R = CN; 3c, R = Ph; 3d, R = CH:CH2; 3e, R = CH:CMe2). Cyclic complex [Ru]-C:C(C6H9)CHCN+ is similarly prepared Protonation of 3b-3e regenerates the corresponding vinylidene complexes. Deprotonation of [Ru]:C:C(Ph)CH2COOMe+ by n-Bu4NOH induces a different type of cyclization and yields the neutral furan complex [cyclic] [Ru]-C:C(Ph)CH:C(O)OMe (4h). The cyclopropenyl complex containing a methoxy substituent cannot be prepared from [Ru]:C:C(Ph)CH2OCH3+ (2i), but F- of n-Bu4NF attacks the Cα of 2i to produce the unstable vinyl complex [Ru]C(F):C(Ph)CH2OCH3. Cyclic complex [Ru]-C:C(Ph)C(CN)OCH3 (9b) was indirectly prepared from the addition of TCNQ to 3b, giving [cyclic] [Ru]:C:C(Ph)CH(CN)TCNQ (6b) followed by methanolysis. Unlike 3, complex 9b is not converted to vinylidene complex, instead, removal of the methoxy substituent by acid gives the cationic cyclopropenylium complex [Ru]-C:C(Ph)C(CN)+. Cyclic complex [Ru]-C:C(Ph)C(COOMe)+ is similarly prepared from 4h via a TCNQ complex followed by a methoxy-substituted complex. In the presence of allyl iodide, opening of the three-membered ring of 3b, followed by a subsequent oxidative coupling reaction, gives a dimeric dicationic product {[Ru]:C:C(Ph)-CHCN}22+ (11). Proton abstraction of 11 by n-Bu4NOH gives the biscyclopropenyl complex {[Ru]-C:C(Ph)CCN}2. Mol. structures of complexes 3b, 4h, 6b, 9b, 11, and [cyclic] [Ru]-C:C(Ph)C(CPh3)CN have been confirmed by x-ray diffraction anal.

IT 178687-62-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(cyclopropenation and related reactions of ruthenium vinylidene complexes)

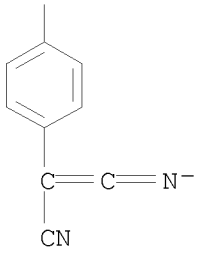
RN 178687-62-2 CAPLUS

CN Ruthenium, (η5-2,4-cyclopentadien-1-yl)[4,4-dicyano-4-[4-(cyanoiminatoethenyl)phenyl]-3-(methoxycarbonyl)-2-phenyl-1-butenylidene]bis(triphenylphosphine)- (9CI) (CA INDEX NAME)

PAGE 1-A

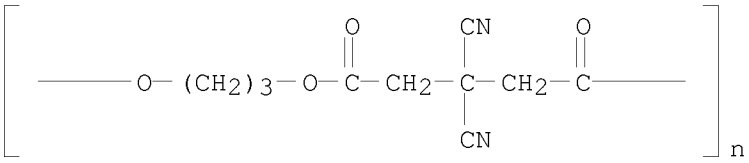


PAGE 2-A

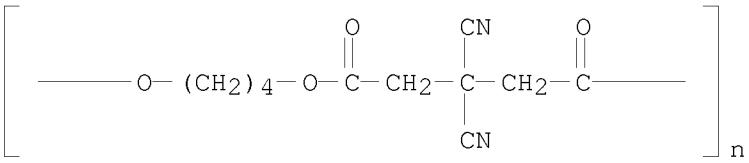


L4 ANSWER 22 OF 68 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1996:6671 CAPLUS
DOCUMENT NUMBER: 124:177091
TITLE: Novel gem-dinitrile functionalized polyesters and polyamides from malononitrile; potential piezoelectric materials
AUTHOR(S): Steadman, Scott; Parrish, Dennis A.; Mathias, Lon J.
CORPORATE SOURCE: Department of Polymer Science, University of Southern Mississippi, Hattiesburg, MS, 39406-0076, USA
SOURCE: Polymer Preprints (American Chemical Society, Division of Polymer Chemistry) (1995), 36(2), 320-1
CODEN: ACPPAY; ISSN: 0032-3934
PUBLISHER: American Chemical Society, Division of Polymer Chemistry

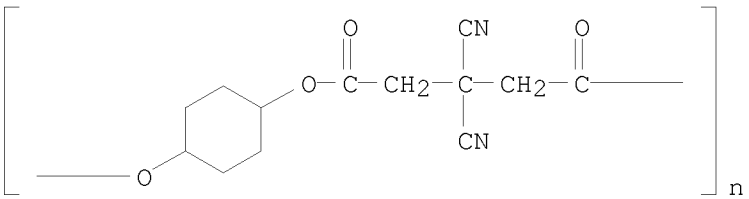
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Novel polyamides and polyesters in which the dinitrile group can potentially align in the same direction as the dipole of the carbonyl groups were synthesized via step growth dialkylation of malononitrile. Diamide and diester monomers facilitated polymerization by the attachment of chlorine to an activated position (α to carbonyl). The polymers, having mol. weight 5000-8000, were characterized by NMR, viscosity and thermal anal.
IT 169893-85-0P 174297-80-4P 174297-82-6P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation of gem-dinitrile functionalized polyesters and polyamides from malononitrile as potential piezoelec. materials)
RN 169893-85-0 CAPLUS
CN Poly[oxy-1,3-propanediyloxy(3,3-dicyano-1,5-dioxo-1,5-pentanediyl)] (9CI) (CA INDEX NAME)



RN 174297-80-4 CAPLUS
CN Poly[oxy-1,4-butanediyloxy(3,3-dicyano-1,5-dioxo-1,5-pentanediyl)] (9CI) (CA INDEX NAME)



RN 174297-82-6 CAPLUS
CN Poly[oxy-1,4-cyclohexanediyloxy(3,3-dicyano-1,5-dioxo-1,5-pentanediyl)] (9CI) (CA INDEX NAME)



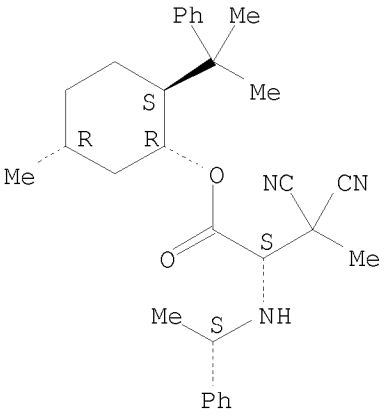
L4 ANSWER 23 OF 68 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1995:900662 CAPLUS

DOCUMENT NUMBER: 124:116317
TITLE: Lanthanum isopropoxide catalyzed addition of activated nucleophiles to imines
AUTHOR(S): Yamamoto, Yoshinori; Fukui, Hiroyuki; Honda, Yoshihiro
CORPORATE SOURCE: Dept. Chem., Tohoku Univ., Sendai, 980-77, Japan
SOURCE: Applied Organometallic Chemistry (1995), 9(5 & 6), 467-71
CODEN: AOCHEX; ISSN: 0268-2605
PUBLISHER: Wiley
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 124:116317

AB The addition of certain activated nucleophiles to activated imines is catalyzed by lanthanum isopropoxide. As activated nucleophiles, methylmaloninitrile and Me 2-cyanopropanoate can be utilized. Imines having an electron-withdrawing group either at the carbon or at the nitrogen atom of the C:N double bond can be used: for example N-toluenesulfonylimines, N-(4-methoxycarbonylphenyl)imines and α-imino esters.

IT 155751-02-3P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(lanthanum isopropoxide catalyzed addition of activated nucleophiles to imines)
RN 155751-02-3 CAPLUS
CN Butanoic acid, 3,3-dicyano-2-[(1-phenylethyl)amino]-, 5-methyl-2-(1-methyl-1-phenylethyl)cyclohexyl ester, [1R-[1α[S*(S*)],2β,5α]]- (9CI) (CA INDEX NAME)

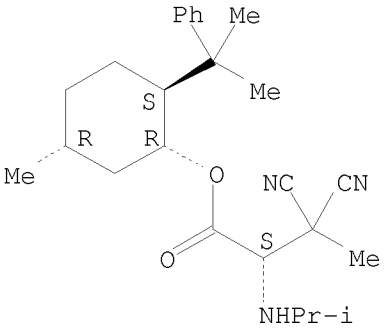
Absolute stereochemistry.



IT 155696-71-2P 155696-72-3P 172880-55-6P
172880-56-7P 173006-24-1P 173006-25-2P
173006-26-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(lanthanum isopropoxide catalyzed addition of activated nucleophiles to imines)
RN 155696-71-2 CAPLUS
CN Butanoic acid, 3,3-dicyano-2-[(1-methylethyl)amino]-, 5-methyl-2-(1-methyl-1-phenylethyl)cyclohexyl ester, [1R-[1α(S*),2β,5α]]-

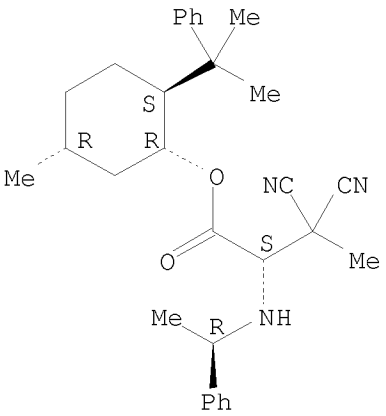
(9CI) (CA INDEX NAME)

Absolute stereochemistry.



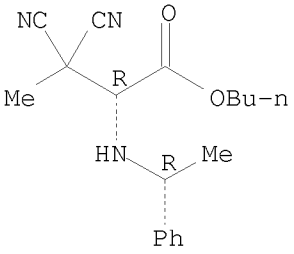
RN 155696-72-3 CAPLUS
CN Butanoic acid, 3,3-dicyano-2-[(1-phenylethyl)amino]-, 5-methyl-2-(1-methyl-1-phenylethyl)cyclohexyl ester, [1R-[1α[S*(R*)],2β,5α]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



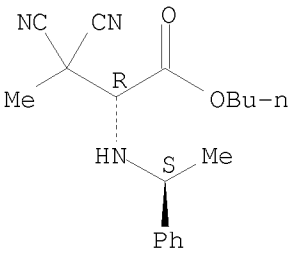
RN 172880-55-6 CAPLUS
CN Butanoic acid, 3,3-dicyano-2-[(1-phenylethyl)amino]-, butyl ester, (R*,R*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



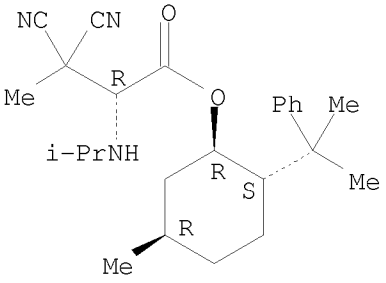
RN 172880-56-7 CAPLUS
CN Butanoic acid, 3,3-dicyano-2-[(1-phenylethyl)amino]-, butyl ester, (R*,S*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



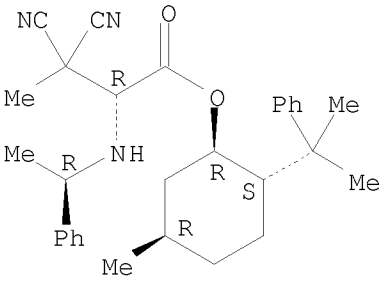
RN 173006-24-1 CAPLUS
CN Butanoic acid, 3,3-dicyano-2-[(1-methylethyl)amino]-, 5-methyl-2-(1-methyl-1-phenylethyl)cyclohexyl ester, [1R-[1α(R*),2β,5α]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



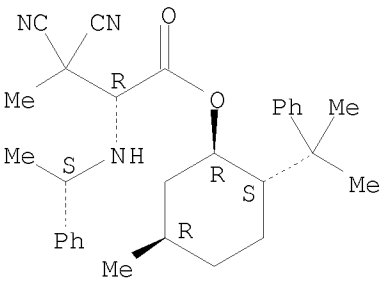
RN 173006-25-2 CAPLUS
CN Butanoic acid, 3,3-dicyano-2-[(1-phenylethyl)amino]-, 5-methyl-2-(1-methyl-1-phenylethyl)cyclohexyl ester, [1R-[1α[R*(R*)],2β,5α]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 173006-26-3 CAPLUS
CN Butanoic acid, 3,3-dicyano-2-[(1-phenylethyl)amino]-, 5-methyl-2-(1-methyl-1-phenylethyl)cyclohexyl ester, [1R-[1α[R*(S*)],2β,5α]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



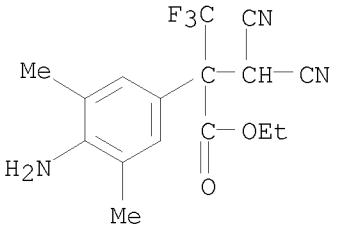
L4 ANSWER 24 OF 68 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1995:845626 CAPLUS
DOCUMENT NUMBER: 124:86769
TITLE: Novel three-component reaction of 1,1-dicyano-2-(trifluoromethyl)ethylenes with primary arylamines and ketones
AUTHOR(S): Tyutin, V. Yu.; Chkanikov, N. D.; Nesterov, V. N.; Antipin, M. Yu.; Struchkov, Yu. T.; Kolomiets, A. F.; Fokin, A. V.
CORPORATE SOURCE: A. N. Nesmeyanov Inst. Organoelem. Compd., Russ. Acad. Sci., Moscow, 117813, Russia
SOURCE: Izvestiya Akademii Nauk, Seriya Khimicheskaya (1993), (3), 552-9
CODEN: IASKEA
PUBLISHER: Nauka
DOCUMENT TYPE: Journal
LANGUAGE: Russian
OTHER SOURCE(S): CASREACT 124:86769
AB 1,1-Dicyano-2,2-bis(trifluoromethyl)ethylene and 3,3-dicyano-2-(trifluoromethyl)acrylates react with primary arylamines in the presence of ketones to form 1,1-aryl-1,4-dihydropyridine derivs. under mild conditions. In this three-component reaction Schiff bases are formed as intermediates. 1,4-Dihydropyridines derivs., which are the products of three-component heterocyclization, were also obtained by interaction of

the corresponding Schiff bases with 1,1-dicyano-2-(trifluoromethyl)ethylenes.

IT 134641-39-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 134641-39-7 CAPLUS

CN Benzeneacetic acid, 4-amino-α-(dicyanomethyl)-3,5-dimethyl-α-(trifluoromethyl)-, ethyl ester (CA INDEX NAME)



L4 ANSWER 25 OF 68 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1995:695727 CAPLUS

DOCUMENT NUMBER: 123:286966

TITLE: Novel gem-dinitrile functionalized polyesters and polyamides from malononitrile; potential piezoelectric materials

AUTHOR(S): Mathias, Lon J.; Parrish, Dennis A.; Steadman, Scott

CORPORATE SOURCE: Department Polymer Science, University Southern Mississippi, Hattiesburg, MS, 39406-0076, USA

SOURCE: Polymer Preprints (American Chemical Society, Division of Polymer Chemistry) (1994), 35(2), 659-60
CODEN: ACPPAY; ISSN: 0032-3934

PUBLISHER: American Chemical Society, Division of Polymer Chemistry

DOCUMENT TYPE: Journal

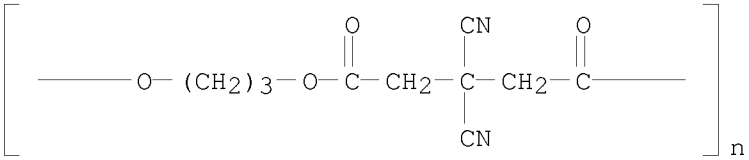
LANGUAGE: English

AB The initial success is described in obtaining a polyester and polyamide in which the dinitrile group net dipole can potentially align in the same direction as the carbonyl groups.

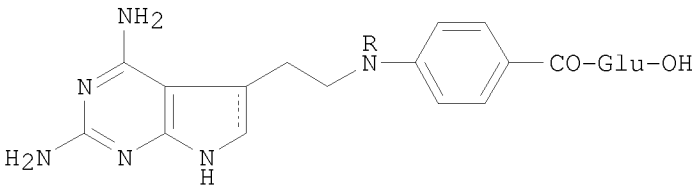
IT 169893-85-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of gem-dinitrile functionalized polyesters and polyamides from malononitrile as potential piezoelec. materials)

RN 169893-85-0 CAPLUS

CN Poly[oxy-1,3-propanediyloxy(3,3-dicyano-1,5-dioxo-1,5-pentanediyl)] (9CI) (CA INDEX NAME)

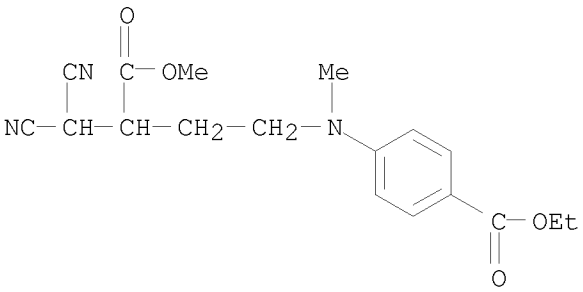


L4 ANSWER 26 OF 68 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1995:440268 CAPLUS
DOCUMENT NUMBER: 123:112653
TITLE: Synthesis and antitumor activity of pyrrolo[2,3-d]pyrimidine antifolates with a bridge chain containing a nitrogen atom
AUTHOR(S): Aso, Kazuyoshi; Hitaka, Takenori; Yukishige, Koichi; Ootsu, Koichiro; Akimoto, Hiroshi
CORPORATE SOURCE: Pharmaceutical Res. Div., Takeda Chem. Industries, Ltd., Osaka, 532, Japan
SOURCE: Chemical & Pharmaceutical Bulletin (1995), 43(2), 256-61
CODEN: CPBTAL; ISSN: 0009-2363
PUBLISHER: Pharmaceutical Society of Japan
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 123:112653
GI

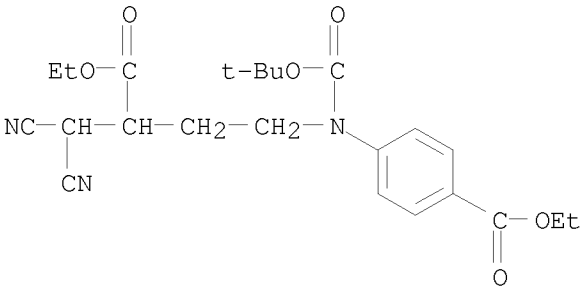


I

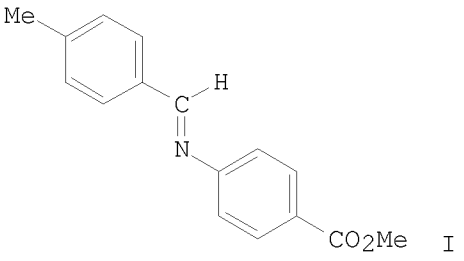
AB Novel pyrrolo[2,3-d]pyrimidine antifolates I (R = H, Me) with a nitrogen atom in the bridge chain between the 2,4-diaminopyrrolo[2,3-d]pyrimidine and phenylene rings were designed and efficiently synthesized. I exhibited more potent inhibitory activities than methotrexate (MTX) against the proliferation of human epidermoid carcinoma KB cells and human non-small cell lung carcinoma A549 cells despite their modest dihydrofolate reductase (DHFR)-inhibitory potency.
IT 133719-38-7P 133719-41-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and antitumor activity of pyrrolo[2,3-d]pyrimidine antifolates with nitrogen-containing bridge chains)
RN 133719-38-7 CAPLUS
CN Benzoic acid, 4-[[4,4-dicyano-3-(methoxycarbonyl)butyl]methylamino]-, ethyl ester (CA INDEX NAME)



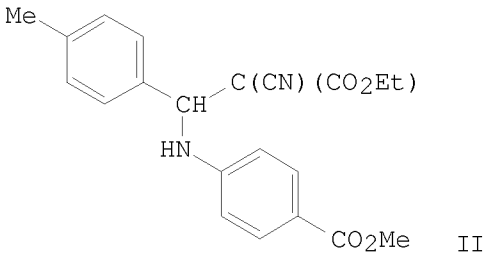
RN 133719-41-2 CAPLUS
CN Benzoic acid, 4-[[4,4-dicyano-3-(ethoxycarbonyl)butyl][(1,1-dimethylethoxy)carbonyl]amino]-, ethyl ester (CA INDEX NAME)



L4 ANSWER 27 OF 68 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1994:434408 CAPLUS
DOCUMENT NUMBER: 121:34408
ORIGINAL REFERENCE NO.: 121:6341a,6342a
TITLE: Transition metal catalyzed addition of certain nucleophiles to imines
AUTHOR(S): Yamamoto, Yoshinori; Kubota, Yasufumi; Honda, Yoshihiro; Fukui, Hiroyuki; Asao, Naoki; Nemoto, Hisao
CORPORATE SOURCE: Faculty of Science, Tohoku University, Sendai, 980, Japan
SOURCE: Journal of the American Chemical Society (1994), 116(7), 3161-2
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 121:34408
GI



I



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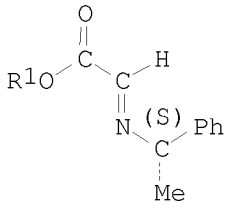
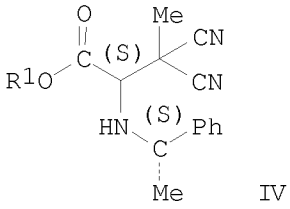


III



IV

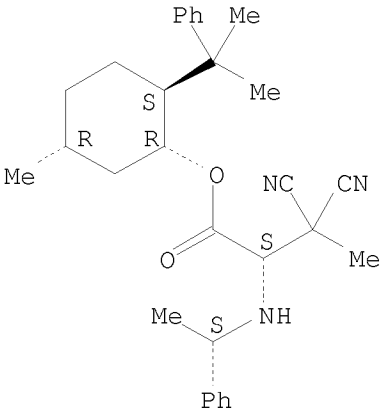
AB Imines react with certain nucleophiles in the presence of catalytic amts. of transition metal complexes to give alkylation products in good yield. Thus, imine (I) was treated with CH(CN)2(CO2Et) in the presence of RhHCO(PPh3)3 in THF solvent to give alkylation product II in 75% yield. A significantly high diastereomeric excess was accomplished by using III [R1 =(-)-8-phenylmenthyl] in which a chiral auxiliary exists at the ester unit. The Ls(O-iso-Pr)3 catalyzed reaction of III with CH(CN)2Me in THF at room temperature gave IV (R1 as above) as the predominant diastereoisomer in a 90:10 ratio; x-ray anal. indicate that the α-carbon to the amino group possesses the S configuration.

IT 155751-02-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, absolute configuration of)

RN 155751-02-3 CAPLUS

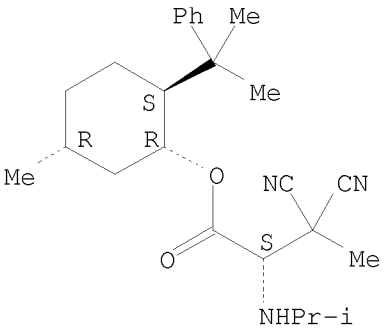
CN Butanoic acid, 3,3-dicyano-2-[(1-phenylethyl)amino]-, 5-methyl-2-(1-methyl-1-phenylethyl)cyclohexyl ester, [1R-[1α[S*(S*)],2β,5α]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



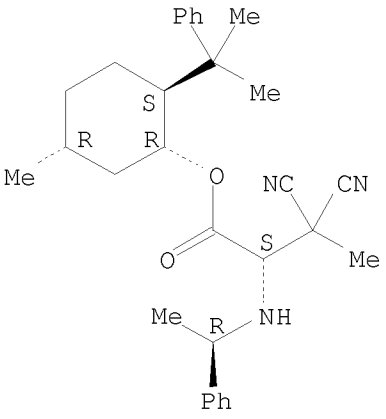
IT 155696-71-2P 155696-72-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, stereoselective)
RN 155696-71-2 CAPLUS
CN Butanoic acid, 3,3-dicyano-2-[(1-methylethyl)amino]-, 5-methyl-2-(1-methyl-1-phenylethyl)cyclohexyl ester, [1R-[1α(S*),2β,5α]]-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.



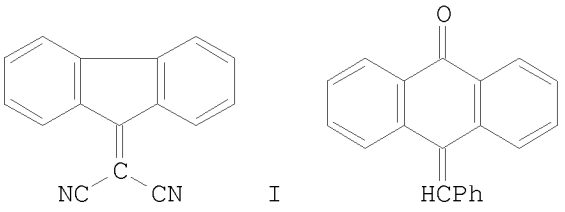
RN 155696-72-3 CAPLUS
CN Butanoic acid, 3,3-dicyano-2-[(1-phenylethyl)amino]-, 5-methyl-2-(1-methyl-1-phenylethyl)cyclohexyl ester, [1R-[1α[S*(R*)],2β,5α]]-
(9CI) (CA INDEX NAME)

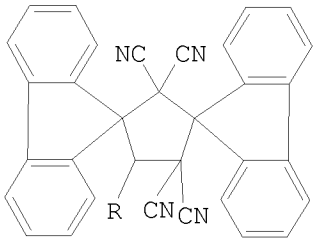
Absolute stereochemistry.



L4 ANSWER 28 OF 68 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1994:269808 CAPLUS
DOCUMENT NUMBER: 120:269808
ORIGINAL REFERENCE NO.: 120:47779a,47782a
TITLE: Wittig reactions of a fluoren-9-ylidene and an anthrone-10-arylidene
AUTHOR(S): Ganoub, Neven A. F.

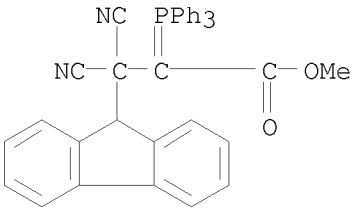
CORPORATE SOURCE: Dep. Pesticide Chem., Natl. Res. Cent., Cairo, Egypt
SOURCE: Phosphorus, Sulfur and Silicon and the Related Elements (1993), 81(1-4), 125-31
CODEN: PSSLEC; ISSN: 1042-6507
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 120:269808
GI



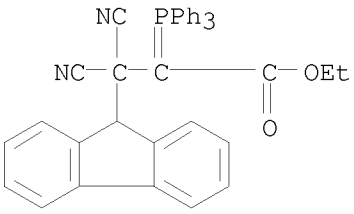


III

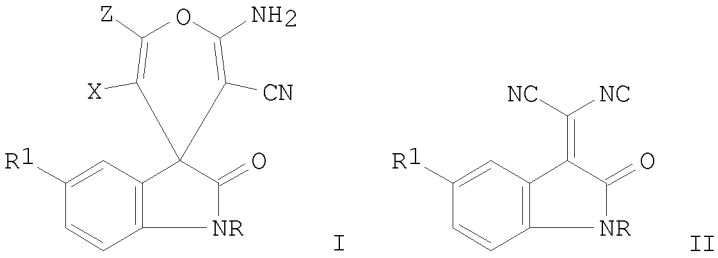
AB The Wittig reactions of fluoren-9-ylidenemalonitrile (I) and 10-benzylideneanthrone (II) with phosphonium ylides Ph3P+CH-CO2R (R = Me, Et) have been investigated. In both cases, unusual reaction products, e.g., bis(9-fluorenyl)cyclopentane III (from I), were isolated and identified on the basis of elemental analyses and spectral studies.
IT 154496-99-8P 154497-00-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and thermal decomposition of)
RN 154496-99-8 CAPLUS
CN 9H-Fluorene-9-propanoic acid, β,β-dicyano-α-(triphenylphosphoranylidene)-, methyl ester (CA INDEX NAME)



RN 154497-00-4 CAPLUS
CN 9H-Fluorene-9-propanoic acid, β,β-dicyano-α-(triphenylphosphoranylidene)-, ethyl ester (CA INDEX NAME)



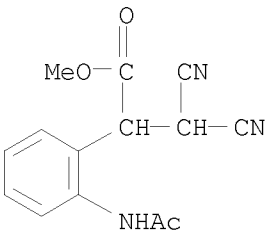
L4 ANSWER 29 OF 68 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1994:244629 CAPLUS
DOCUMENT NUMBER: 120:244629
ORIGINAL REFERENCE NO.: 120:43353a,43356a
TITLE: Synthesis of spiro indolin-2-one derivatives
AUTHOR(S): El-Ahl, Abdel Aziz S.; Afeefy, Hussein; Metwally, Mohamed Abbas
CORPORATE SOURCE: Fac. Sci., Mansoura Univ., Mansoura, Egypt
SOURCE: Journal of Chemical Research, Synopses (1994), (1), 14-15
CODEN: JRPSDC; ISSN: 0308-2342
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 120:244629
GI



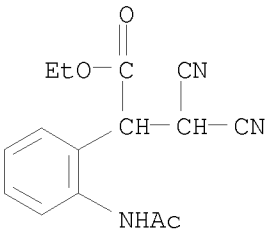
I

II

AB Title compds. I were prepared by heating dicyanomethyleneindolinones II (R = H, R1 = H, Me; R = Me, Ac, R1 = H) with active methylene compds., XCH2COZ (X = Ac, Z = OEt, Me; X = cyano, Z = Ph).
IT 154379-70-1P 154379-71-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 154379-70-1 CAPLUS
CN Benzeneacetic acid, 2-(acetylamino)-α-(dicyanomethyl)-, methyl ester (CA INDEX NAME)



RN 154379-71-2 CAPLUS
CN Benzeneacetic acid, 2-(acetylamino)-α-(dicyanomethyl)-, ethyl ester (CA INDEX NAME)



L4 ANSWER 30 OF 68 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1993:213100 CAPLUS
DOCUMENT NUMBER: 118:213100
ORIGINAL REFERENCE NO.: 118:36739a,36742a
TITLE: Preparation of tricyclic fused pyrimidine compounds
INVENTOR(S): Akimoto, Hiroshi; Otsu, Koichiro; Miwa, Tetsuo
PATENT ASSIGNEE(S): Takeda Chemical Industries, Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 25 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 04211063	A	19920803	JP 1991-65613	19910305 <--
PRIORITY APPLN. INFO.:			JP 1990-54620 A1	19900305

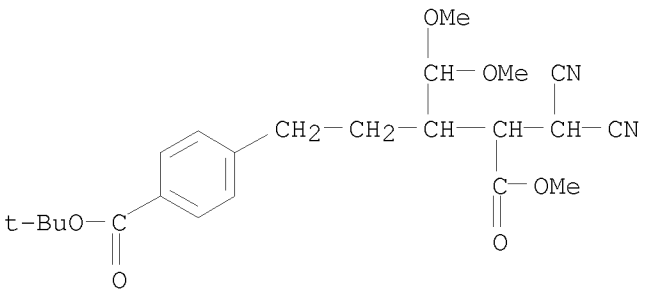
OTHER SOURCE(S): MARPAT 118:213100
GI For diagram(s), see printed CA Issue.
AB The title compds. [I; Q1 = H, halo, radical linked through C, N, O, or S; one of Q2 and Q3 = N, the other = N, CH; Y = N, CR1 (wherein R1 = H, hydrocarbyl), methylidyne; Z = C2-5 bivalent radical containing optional substituents; ring A1, A2 = (substituted) 5-7-membered ring; B = (substituted) cyclic radical, etc.], useful as antitumor agents with high selectivity, are prepared Cyclocondensation of 1.181 g ester II (preparation given) with 314 mg guanidine HCl and Me3COK in Me3COH gave 1.02 g pyrrolopyrimidine III, which (1.010 g) was treated with borane-THF complex in THF at 0° and then at 50°, the solution cooled and stirred with HOAc-MeOH at room temperature to give 542 mg IV. The preferred doses of I

are 2.0-500 mg/kg-day orally and 1.0-200 mg/kg injection.

IT 147239-87-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, in preparation of antitumor agent)

RN 147239-87-0 CAPLUS

CN Benzenepentanoic acid, α-(dicyanomethyl)-β-(dimethoxymethyl)-4-[(1,1-dimethylethoxy)carbonyl]-, methyl ester (CA INDEX NAME)



L4 ANSWER 31 OF 68 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1993:124655 CAPLUS

DOCUMENT NUMBER: 118:124655

ORIGINAL REFERENCE NO.: 118:21621a,21624a

TITLE: Wittig reaction of 1-(dicyanomethylene)acenaphthen-2-one

AUTHOR(S): Abdou, Wafaa M.; Ganoub, Neven A. F.

CORPORATE SOURCE: Natl. Res. Cent., Cairo, Egypt

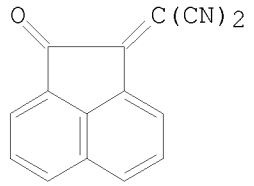
SOURCE: Heteroatom Chemistry (1992), 3(2), 133-7
CODEN: HETCE8; ISSN: 1042-7163

DOCUMENT TYPE: Journal

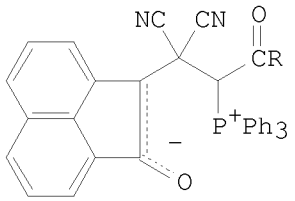
LANGUAGE: English

OTHER SOURCE(S): CASREACT 118:124655

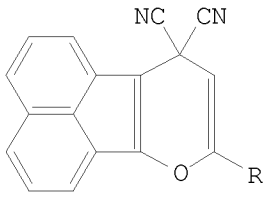
GI



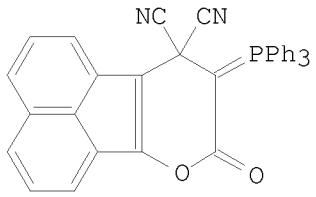
I



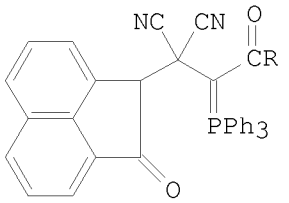
II



III



IV



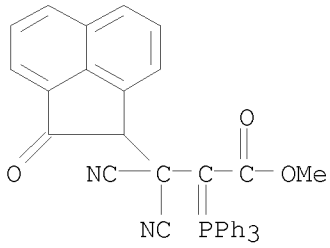
V

AB The Wittig reactions of title compound I with alkoxycarbonylmethylenetriphen ylphosphoranes Ph3P+C-HCOR (R = OMe, OEt) were investigated and the reaction products zwitterion II and heterocycles III and IV were isolated. Reaction of I with benzoylmethylenetriphenylphosphorane Ph3P+C-HCOPh proceeded only at high temperature, yielding V and III (R = Ph). Mechanisms accounting for the formation of the adducts are discussed. Wittig olefination of several products was studied.

IT 145882-80-0P 145882-83-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

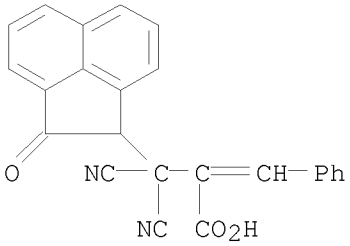
RN 145882-80-0 CAPLUS

CN 1-Acenaphthylenepropanoic acid, β,β-dicyano-1,2-dihydro-2-oxo-α-(triphenylphosphoranylidene)-, methyl ester (CA INDEX NAME)

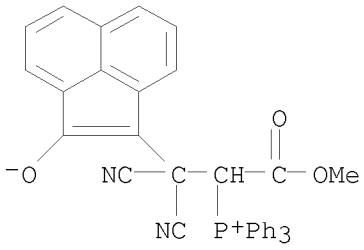


RN 145882-83-3 CAPLUS

CN 1-Acenaphthylenepropanoic acid, β,β-dicyano-1,2-dihydro-2-oxo-α-(phenylmethylene)- (CA INDEX NAME)



IT 145882-82-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, Wittig olefination, and thermal intramol. cyclocondensation of)
RN 145882-82-2 CAPLUS
CN Phosphonium, [2,2-dicyano-2-(2-hydroxy-1-acenaphthylenyl)-1-(methoxycarbonyl)ethyl]triphenyl-, inner salt (CA INDEX NAME)



L4 ANSWER 32 OF 68 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1993:29863 CAPLUS
DOCUMENT NUMBER: 118:29863
ORIGINAL REFERENCE NO.: 118:5361a,5364a
TITLE: Silver halide photographic material containing a compound which releases photographically useful species upon development
INVENTOR(S): Asatake, Atsushi
PATENT ASSIGNEE(S): Konica Co., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 19 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

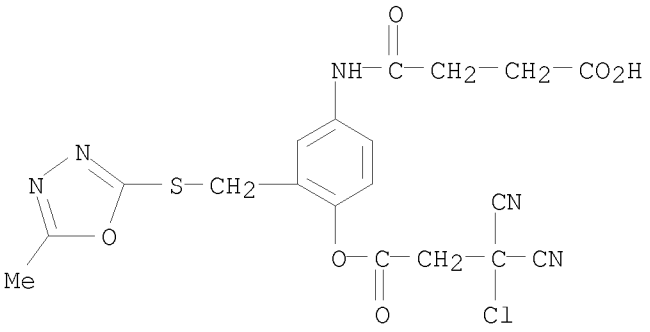
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 04177243	A	19920624	JP 1990-305540	19901110 <--

PRIORITY APPLN. INFO.: JP 1990-305540 19901110
AB The photog. material contains a compound CRR1R2C(R3R4)mZ(Z1)nPUG (R = leaving group released by nucleophilic substitution; R1,R2,R3,R4 = H,

aliphatic, aromatic, heterocyclic or electron-attracting group; Z = electron-attracting group; Z1 = timing group to be subjected to break and release PUG: PUG = photog. useful group; m,n = 0, 1). The photog. material has good storage stability, while upon development, it releases the PUGs at a proper reaction rate even in developer solution of relatively low pH.

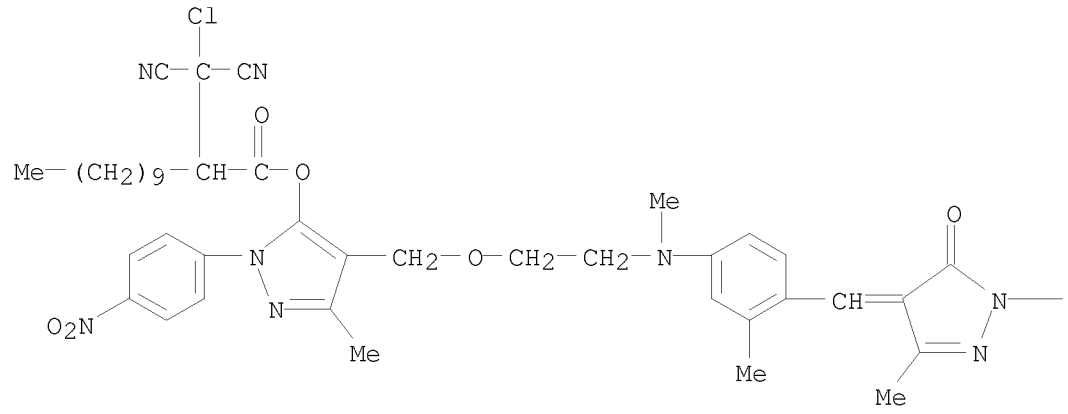
IT 144896-71-9 145059-42-3
RL: USES (Uses)
(photog. useful group-releasing, in processing)

RN 144896-71-9 CAPLUS
CN Butanoic acid, 4-[[4-(3-chloro-3,3-dicyano-1-oxopropoxy)-3-[[(5-methyl-1,3,4-oxadiazol-2-yl)thio]methyl]phenyl]amino]-4-oxo- (CA INDEX NAME)

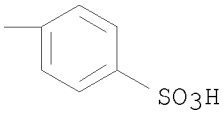


RN 145059-42-3 CAPLUS
CN Dodecanoic acid, 2-(chlorodicyanomethyl)-, 4-[[2-[[4-[[1,5-dihydro-3-methyl-5-oxo-1-(4-sulfophenyl)-4H-pyrazol-4-ylidene]methyl]-3-methylphenyl]methylamino]ethoxy]methyl]-3-methyl-1-(4-nitrophenyl)-1H-pyrazol-5-yl ester, monopotassium salt (9CI) (CA INDEX NAME)

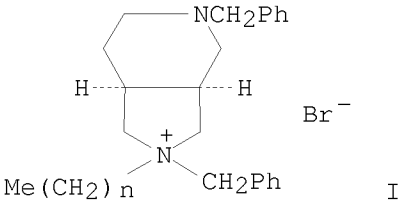
PAGE 1-A



● K



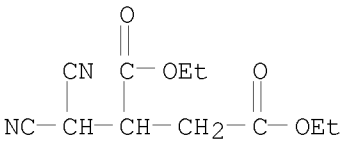
L4 ANSWER 33 OF 68 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1992:174018 CAPLUS
DOCUMENT NUMBER: 116:174018
ORIGINAL REFERENCE NO.: 116:29451a,29454a
TITLE: Synthesis and structure-antimicrobial activity relationships of quaternary ammonium derivatives of perhydropyrrolo-[3,4-c]pyridine
AUTHOR(S): Altomare, C.; Carotti, A.; Casini, G.; Cellamare, S.; Ferappi, M.; Vitali, C.
CORPORATE SOURCE: Dip. Farm. Chim., Univ. Bari, Bari, I-70125, Italy
SOURCE: Arzneimittel-Forschung (1992), 42(2), 152-5
CODEN: ARZNAD; ISSN: 0004-4172
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 116:174018
GI



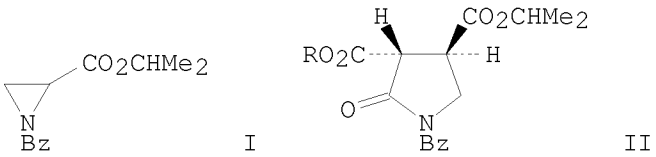
I

AB A homologous series of perhydropyrrolo[3,4-c]pyridine quaternary ammonium derivs. I (n = 5, 7, 9-13,15) was synthesized from EtO2CCH2CH(CO2Et)CH(CN)2 and tested for in vitro antibacterial activity against different gram-pos. and gram-neg. bacteria. All I were more potent than the reference compound, benzalkonium chloride. Antibacterial activity, expressed as log 1/MIC, was linearly related to lipophilicity up to C13-C14 homologs, where a break in the linear relationship was observed

IT 82584-86-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(hydrogenation-intramol. cyclocondensation of)
RN 82584-86-9 CAPLUS
CN Butanedioic acid, (dicyanomethyl)-, diethyl ester (9CI) (CA INDEX NAME)



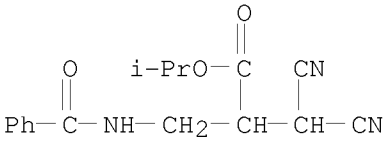
L4 ANSWER 34 OF 68 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1992:83465 CAPLUS
DOCUMENT NUMBER: 116:83465
ORIGINAL REFERENCE NO.: 116:14203a,14206a
TITLE: The regioselectivity of the ring opening of 1-activated or nonactivated 2-alkoxycarbonyl or 2-cyanoaziridines by carbanions of the dicarbonyl compounds
AUTHOR(S): Bouayad, Zoheir; Chanet-Ray, Josette; Ducher, S.; Vessiere, Roger
CORPORATE SOURCE: Ec. Natl. Super. Chim. Clermont-Ferrand, Univ. Blaise Pascal, Aubiere, 63177, Fr.
SOURCE: Journal of Heterocyclic Chemistry (1991), 28(7), 1757-67
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



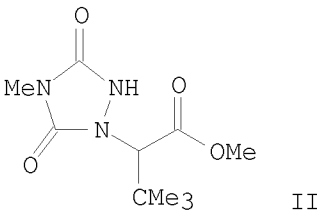
I II

AB Aziridines, e.g. I, reacted with carbanions of dicarbonyl compds., e.g. RO2CCH2CO2R (R = Me, Et, CHMe2), to give ring opened products and/or ring enlarged products, e.g. (RO2C)2CHCH2CH(NHBz)CO2CHMe2, (RO2C)2CHCH(CO2CHMe2)CH2NHBz, and pyrrole II. The regioselectivity depends on several factors. The Ph group on C-3 favors C-3-N bond cleavage, whereas C-2-N bond cleavage is predominant with C-3 substituted or C-2-H aziridines. Cyanoaziridines are predominantly cleaved at C-3-N.
IT 138478-35-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 138478-35-0 CAPLUS

CN Propanoic acid, 2-[(benzoylamino)methyl]-3,3-dicyano-, 1-methylethyl ester (CA INDEX NAME)



L4 ANSWER 35 OF 68 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1991:680104 CAPLUS
DOCUMENT NUMBER: 115:280104
ORIGINAL REFERENCE NO.: 115:47607a,47610a
TITLE: E/Z isomerization, solvolysis, addition, and cycloaddition reactions of (E)-tert-butylketene methyl tert-butyldimethylsilyl acetal
AUTHOR(S): Adam, Waldemar; Wang, Xiaoheng
CORPORATE SOURCE: Inst. Org. Chem., Univ. Wuerzburg, Wuerzburg, D-8700, Germany
SOURCE: Journal of Organic Chemistry (1991), 56(26), 7244-50
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 115:280104
GI



II

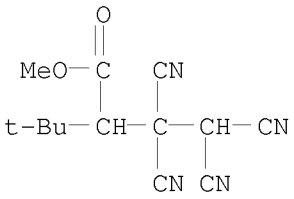
AB In the presence of catalytic amts. of CF3COMe or CF3COCF3, the silyl ketene acetal Me3CCH:C(OMe)OSiMe2CMe3 (E-I) was isomerized into its Z isomer (Z/E ratio 90:10). For this novel E/Z isomerization a mechanism is proposed in which addition and reelimination of the fluoro ketone through a 1,4-dipolar intermediate operates. With the protic nucleophiles MeOH, CF3CH2OH, or PhOH, the ketene acetal E-I afforded the ortho esters Me3CCH2C(OMe)(OR)OSiMe2CMe3 (R = Me, CF3CH2, Ph) as addition products, while AcOH, CF3CO2H, or H2O led to Me pivalate as the solvolysis product. This chemical is readily explained through protonation of the ketene acetal E-I to generate the corresponding carbenium ion. At low temperature the reaction with TCNE gave the silylketene imine as labile cycloadduct, which underwent desilylation on workup to give the TCNE-incorporated ester

(NC)2CHC(CN)2CH(CMe2)C(O)OMe; the latter eliminated hydrogen cyanide at room temperature to give the ene ester. With MTAD the labile silyl ene product was obtained initially, which underwent silyl migration to give N-silylated urazole; final desilylation led to the stable urazole II. Also, for the ene reactions of TCNE and MTAD with the silyl ketene acetal E-I, intervention of a 1,4-dipolar intermediate is proposed.

IT 136911-64-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and hydrogen cyanide elimination of)

RN 136911-64-3 CAPLUS

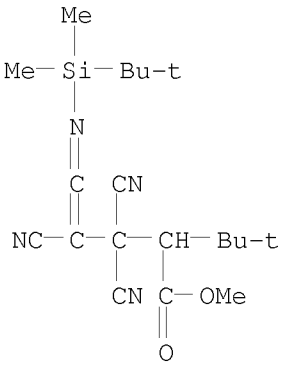
CN Butanoic acid, 3,3,4,4-tetracyano-2-(1,1-dimethylethyl)-, methyl ester (9CI) (CA INDEX NAME)



IT 136911-63-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 136911-63-2 CAPLUS

CN 4-Pentenoic acid, 3,3,4-tricyano-2-(1,1-dimethylethyl)-5-[[(1,1-dimethylethyl)dimethylsilyl]imino]-, methyl ester (CA INDEX NAME)



L4 ANSWER 36 OF 68 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1991:608100 CAPLUS

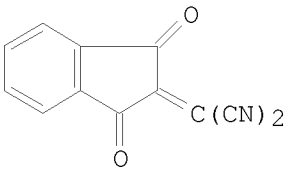
DOCUMENT NUMBER: 115:208100

ORIGINAL REFERENCE NO.: 115:35517a,35520a

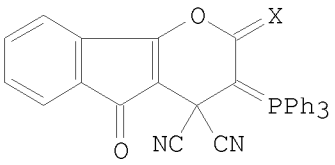
TITLE: Chemistry of phosphorus ylides. 10. Reaction with phosphacumulenes. IV. Synthesis of pyran, phosphoranylidene, oxaphosphorin and oxazaphosphorin from the reaction of 1,3-dioxo-Δ2,α-indanmalononitrile with phosphoranes and

iminophosphoranes

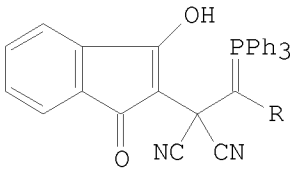
AUTHOR(S): Soliman, Fouad M.; Said, Medhat M.
CORPORATE SOURCE: Natl. Res. Cent., Cairo, Egypt
SOURCE: Phosphorus, Sulfur and Silicon and the Related Elements (1991), 61(3-4), 335-40
CODEN: PSSLEC; ISSN: 1042-6507
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 115:208100
GI



I



II

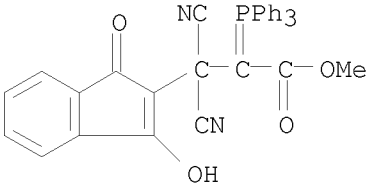


III

AB 1,3-Dioxo-Δ2,α-indanmalononitrile (I) reacts with the active ketenylidene- and thioketenylidenetriphenylphosphoranes Ph3P:C:C:X (X = O, S, resp.) to give the corresponding pyrans II (X = O, S). The reaction of II with 4-O2NC6H4CHO proceeds according to the Wittig reaction to give the resp. methylidene derivs. On the other hand, phosphoranylidenes III (R = acyl, alkoxycarbonyl) were isolated from the reaction of stable phosphoranes Ph3P:CHR with I. Moreover, an oxaphosphorin and oxazaphosphorin were prepared from the reaction of I with the phosphorane Ph3P:CPh2 and the iminophosphorane Ph3P:NCO2Et, resp.

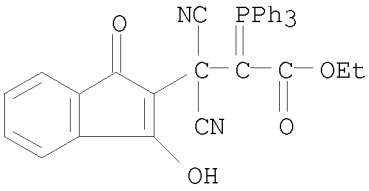
IT 136829-50-0P 136848-91-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 136829-50-0 CAPLUS
CN 1H-Indene-2-propanoic acid, β,β-dicyano-3-hydroxy-1-oxo-α-(triphenylphosphoranylidene)-, methyl ester (CA INDEX NAME)

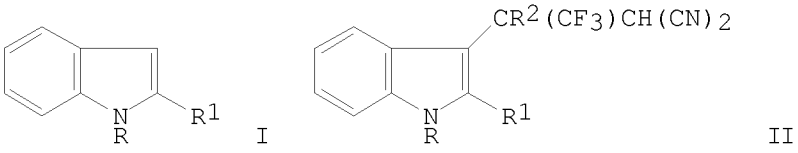


RN 136848-91-4 CAPLUS
CN 1H-Indene-2-propanoic acid, β,β-dicyano-3-hydroxy-1-oxo-α-

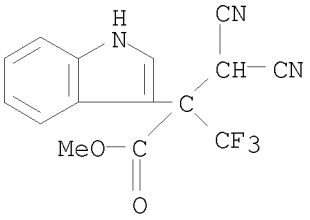
(triphenylphosphoranylidene)-, ethyl ester (CA INDEX NAME)



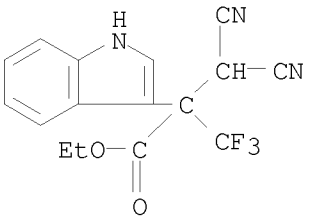
L4 ANSWER 37 OF 68 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1991:492003 CAPLUS
DOCUMENT NUMBER: 115:92003
ORIGINAL REFERENCE NO.: 115:15823a,15826a
TITLE: C-Alkylation of indoles with 1,1-bis(trifluoromethyl)-2,2-dicyanoethylene and 2-trifluoromethyl-3,3-dicyanoacrylic acid esters
AUTHOR(S): Chkanikov, N. D.; Komarov, K. V.; Tyutin, V. Yu.; Kolomiets, A. F.; Fokin, A. V.
CORPORATE SOURCE: Inst. Elementoorg. Soedin. im. Nesmeyanova, Moscow, USSR
SOURCE: Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya (1991), (5), 1193-5
CODEN: IASKA6; ISSN: 0002-3353
DOCUMENT TYPE: Journal
LANGUAGE: Russian
OTHER SOURCE(S): CASREACT 115:92003
GI



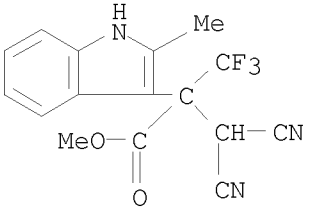
AB The indole derivs. I (R = H, Me; R1 = H, Me, Ph) were alkylated with (NC)2C:CR2CF3 (R2 = CF3, CO2Me, CO2Et) to give the corresponding dicyanoethyl derivs. II.
IT 135578-14-2P 135578-15-3P 135578-17-5P
135578-18-6P 135578-19-7P 135578-20-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 135578-14-2 CAPLUS
CN 1H-Indole-3-acetic acid, α-(dicyanomethyl)-α-(trifluoromethyl)-, methyl ester (CA INDEX NAME)



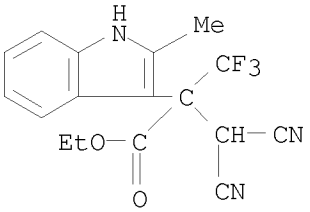
RN 135578-15-3 CAPLUS
CN 1H-Indole-3-acetic acid, α-(dicyanomethyl)-α-(trifluoromethyl)-, ethyl ester (CA INDEX NAME)



RN 135578-17-5 CAPLUS
CN 1H-Indole-3-acetic acid, α-(dicyanomethyl)-2-methyl-α-(trifluoromethyl)-, methyl ester (CA INDEX NAME)

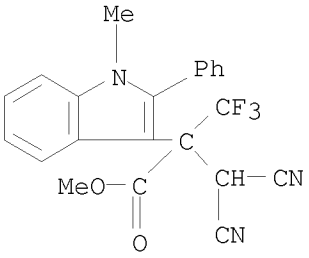


RN 135578-18-6 CAPLUS
CN 1H-Indole-3-acetic acid, α-(dicyanomethyl)-2-methyl-α-(trifluoromethyl)-, ethyl ester (CA INDEX NAME)

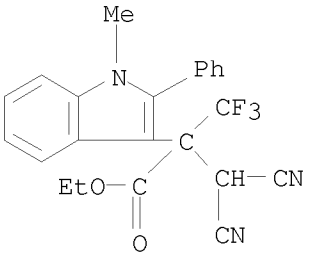


RN 135578-19-7 CAPLUS

CN 1H-Indole-3-acetic acid, α-(dicyanomethyl)-1-methyl-2-phenyl-α-(trifluoromethyl)-, methyl ester (CA INDEX NAME)



RN 135578-20-0 CAPLUS
CN 1H-Indole-3-acetic acid, α-(dicyanomethyl)-1-methyl-2-phenyl-α-(trifluoromethyl)-, ethyl ester (CA INDEX NAME)



L4 ANSWER 38 OF 68 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1991:471633 CAPLUS
DOCUMENT NUMBER: 115:71633
ORIGINAL REFERENCE NO.: 115:12391a,12394a
TITLE: Preparation of pyrrolopyrimidines as antitumor agents
INVENTOR(S): Akimoto, Hiroshi; Hitaka, Takenori
PATENT ASSIGNEE(S): Takeda Chemical Industries, Ltd., Japan
SOURCE: Eur. Pat. Appl., 27 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 418924	A2	19910327	EP 1990-118202	19900921 <--
EP 418924	A3	19911023		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
JP 03173890	A	19910729	JP 1990-249615	19900918 <--
CA 2025830	A1	19910322	CA 1990-2025830	19900920 <--
US 5354754	A	19941011	US 1993-46917	19930414 <--
PRIORITY APPLN. INFO.:			JP 1989-245998 A	19890921
			US 1990-585950 B1	19900921

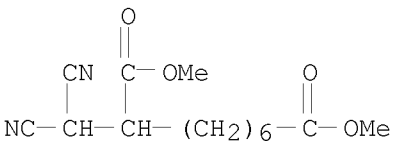
OTHER SOURCE(S): MARPAT 115:71633
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

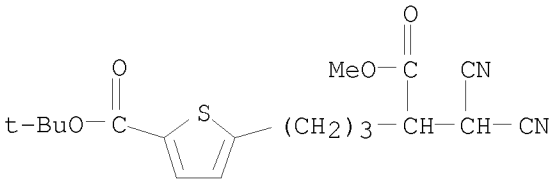
AB Pyrrolopyrimidines [I; R1, R2 = H, ester residue; X = NH2, OH, SH; Y = H, OH; Z = (substituted) C2-4 divalent radical; Z1 = (substituted) divalent heterocycle residue, alkylene; dotted line indicates saturation or unsatn] are prepared Acetal II (1.32 g) (preparation given) was dissolved in CF3CO2H containing H2O with stirring at room temperature to give quant. salt III, which was dissolved with di-Et glutamate HCl in DMF and the solution was treated with 0.514 g H2NP(O)(OEt)2 and Et3N in DMF at room temperature to give 1.11 g diester IV (R1 = R2 = Et) (V). Saponification of 1.05 g V in THF gave 0.826 g acid IV (R1 = R2 = H), which showed IC50 of 0.00043 μg/mL against human epidermoid carcinoma KB cells.

IT 135110-11-1P 135111-93-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, in preparation of antitumor agent)

RN 135110-11-1 CAPLUS
CN Nonanedioic acid, 2-(dicyanomethyl)-, dimethyl ester (9CI) (CA INDEX NAME)



RN 135111-93-2 CAPLUS
CN 2-Thiophenepentanoic acid, α-(dicyanomethyl)-5-[(1,1-dimethylethoxy)carbonyl]-, methyl ester (CA INDEX NAME)

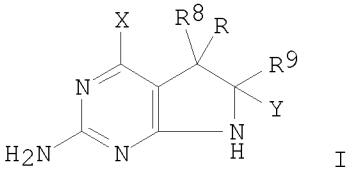


L4 ANSWER 39 OF 68 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1991:429914 CAPLUS
DOCUMENT NUMBER: 115:29914
ORIGINAL REFERENCE NO.: 115:5281a,5284a

TITLE: Preparation of N-[[(pyrrolopyrimidinylethyl)amino]benzoyl]glutamates and analogs as antitumor agents
INVENTOR(S): Akimoto, Hiroshi; Hitaka, Takenori; Miwa, Tetsuo
PATENT ASSIGNEE(S): Takeda Chemical Industries, Ltd., Japan
SOURCE: Eur. Pat. Appl., 51 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 400562	A1	19901205	EP 1990-110131	19900529 <--
EP 400562	B1	19960821		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
JP 04009382	A	19920114	JP 1990-136345	19900525 <--
JP 3015957	B2	20000306		
CA 2017604	A1	19901129	CA 1990-2017604	19900528 <--
AT 141603	T	19960915	AT 1990-110131	19900529 <--

PRIORITY APPLN. INFO.: JP 1989-135642 A 19890529
JP 1989-246209 A 19890920
JP 1990-93370 A 19900409
OTHER SOURCE(S): MARPAT 115:29914
GI



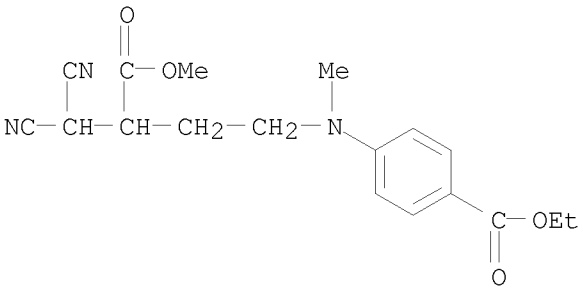
I

AB The title compds. [I; R = (CR1R2)iZ1(CR4R5)jZ2CONHCH(CO2R6)CH2CH2CO2R7; R1, R2, R4, R5 = H, hydrocarbyl, bond; R6, R7 = H, alkyl, (un)substituted Ph, PhCH2; R8, R9 = H; R8R9 = bond; X = NH2, OH, SH; Y = H, OH; Z1 = O, SOn, (alkyl)imino, etc.; Z2 = (un)substituted alkylene, divalent cyclic group; i,j = 0-3 (i + j = 1-3); n = 0-2] were prepared Thus, 4-(EtO2C)C6H4NMeCH2CH2CH(CO2Me)CH(CN)2 (preparation given) was cyclocondensed with guanidine and the product reduced to give, as 1 of 2 products, anilinoethylpyrrolopyrimidine I [R = CH2CH2NMeC6H4(COR10)-4; R8R9 = bond, X = NH2, Y = H] (II; R10 = OEt) which was condensed with di-Et L-glutamate to give, after saponification, L-II [R10 = NHCH(CO2H)CH2CH2CO2H]. The latter had IC50 of 0.0013 μM against human epidermoid carcinoma KB cell growth in vitro.

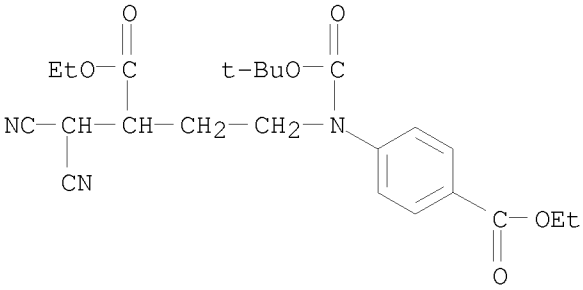
IT 133719-38-7P 133719-41-2P 133719-45-6P
133719-47-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, in preparation of antitumor agents)

RN 133719-38-7 CAPLUS
CN Benzoic acid, 4-[[4,4-dicyano-3-(methoxycarbonyl)butyl]methylamino]-,

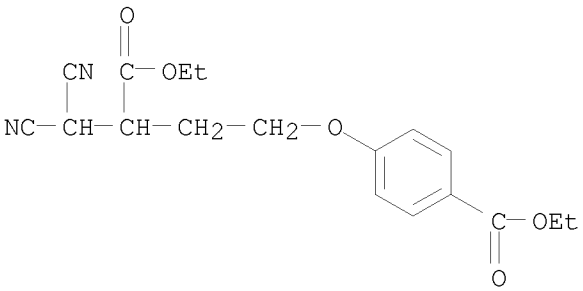
ethyl ester (CA INDEX NAME)



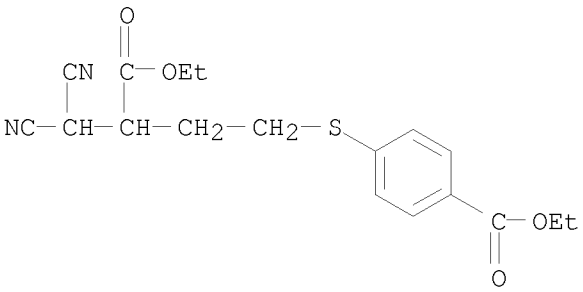
RN 133719-41-2 CAPLUS
CN Benzoic acid, 4-[[4,4-dicyano-3-(ethoxycarbonyl)butyl][(1,1-dimethylethoxy)carbonyl]amino]-, ethyl ester (CA INDEX NAME)



RN 133719-45-6 CAPLUS
CN Benzoic acid, 4-[4,4-dicyano-3-(ethoxycarbonyl)butoxy]-, ethyl ester (CA INDEX NAME)



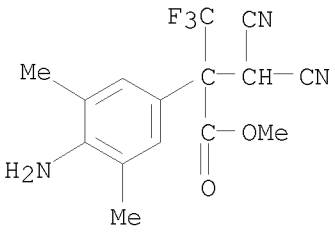
RN 133719-47-8 CAPLUS
CN Benzoic acid, 4-[[4,4-dicyano-3-(ethoxycarbonyl)butyl]thio]-, ethyl ester (CA INDEX NAME)



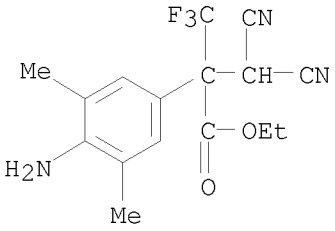
L4 ANSWER 40 OF 68 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1991:429194 CAPLUS
DOCUMENT NUMBER: 115:29194
ORIGINAL REFERENCE NO.: 115:5133a,5136a
TITLE: Synthesis of esters of 3,3-dicyano-2-(trifluoromethyl)acrylic acid and their reactions with aryl amines
AUTHOR(S): Tyutin, V. Y.; Chkanikov, N. D.; Kolomiets, A. F.; Fokin, A. V.
CORPORATE SOURCE: Inst. Organoelem. Compd., Moscow, 117813, USSR
SOURCE: Journal of Fluorine Chemistry (1991), 51(3), 323-34
CODEN: JFLCAR; ISSN: 0022-1139
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 115:29194
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

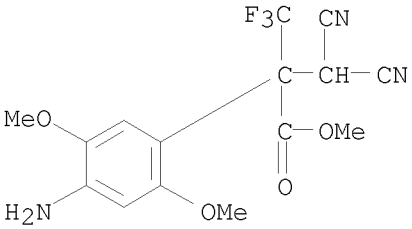
AB Title acrylates (NC)2C:C(CF3)CO2R (I; R = Me, Et) were prepared by the condensation of CH2(CN)2 with CF3COCO2R in presence of ZnCl2. Reaction of I with aromatic amines was investigated. Thus, 2,6-dimethylaniline reacted with I in CHCl3 to give adduct II. 2,5-Dimethoxyaniline, and Ph2NH gave similar adducts. o- And m-C6H4(NH2)2 reacted with I to give cyclocondensation products, quinoxalinone III and indoline IV resp. 4-R1C6H4NHNH2 (R1 = H, NO2) gave pyrazolines V on cyclocondensation with I. Reaction of I with 3-aminopyrazole gave pyrazolopyridines VI.
IT 134641-38-6P 134641-39-7P 134641-40-0P
134641-41-1P 134641-42-2P 134641-43-3P
134641-44-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 134641-38-6 CAPLUS
CN Benzeneacetic acid, 4-amino-α-(dicyanomethyl)-3,5-dimethyl-α-(trifluoromethyl)-, methyl ester (CA INDEX NAME)



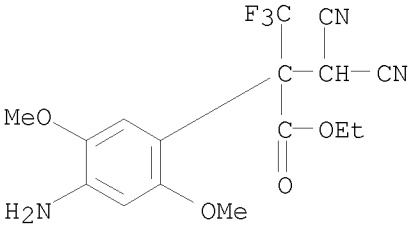
RN 134641-39-7 CAPLUS
CN Benzeneacetic acid, 4-amino-α-(dicyanomethyl)-3,5-dimethyl-α-(trifluoromethyl)-, ethyl ester (CA INDEX NAME)



RN 134641-40-0 CAPLUS
CN Benzeneacetic acid, 4-amino-α-(dicyanomethyl)-2,5-dimethoxy-α-(trifluoromethyl)-, methyl ester (CA INDEX NAME)

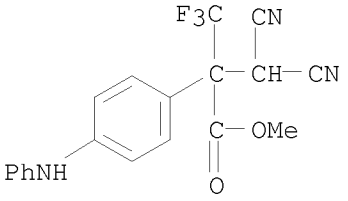


RN 134641-41-1 CAPLUS
CN Benzeneacetic acid, 4-amino-α-(dicyanomethyl)-2,5-dimethoxy-α-(trifluoromethyl)-, ethyl ester (CA INDEX NAME)

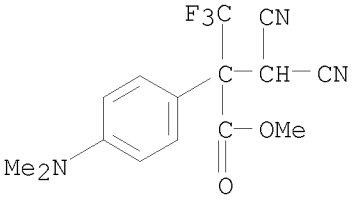


RN 134641-42-2 CAPLUS

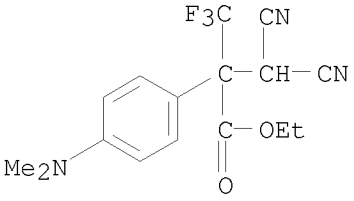
CN Benzeneacetic acid, α-(dicyanomethyl)-4-(phenylamino)-α-(trifluoromethyl)-, methyl ester (CA INDEX NAME)



RN 134641-43-3 CAPLUS
CN Benzeneacetic acid, α-(dicyanomethyl)-4-(dimethylamino)-α-(trifluoromethyl)-, methyl ester (CA INDEX NAME)

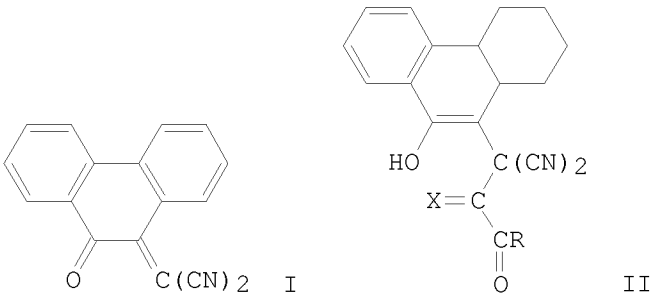


RN 134641-44-4 CAPLUS
CN Benzeneacetic acid, α-(dicyanomethyl)-4-(dimethylamino)-α-(trifluoromethyl)-, ethyl ester (CA INDEX NAME)



L4 ANSWER 41 OF 68 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1991:247080 CAPLUS
DOCUMENT NUMBER: 114:247080
ORIGINAL REFERENCE NO.: 114:41709a,41712a
TITLE: Reaction of α,β-unsaturated nitriles with phosphorus ylides
AUTHOR(S): Abdou, Wafaa M.; Ganoub, Neven A. F.
CORPORATE SOURCE: Natl. Res. Cent., Dokki, Egypt
SOURCE: Chemistry & Industry (London, United Kingdom) (1991), (6), 217-18
CODEN: CHINAG; ISSN: 0009-3068
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 114:247080

GI

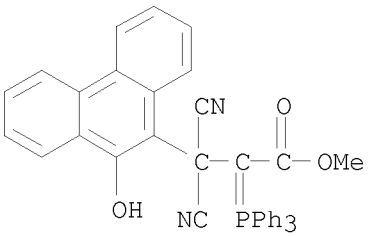


AB Reaction of unsatd. nitrile I with ROCC-HP+Ph3 (R = OMe, OEt, Ph) in benzene at 25° gave 75-80% addition products II (X = PPh3). On heating II (X = PPh3) to 200° they underwent an intramol. Wittig reaction to give arenopyrans III. Heating phosphorane II (R = OMe, X = PPh3) with BzH gave II (X = CHPh).

IT 133973-19-0P 133973-20-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and intramol. Wittig reaction of)

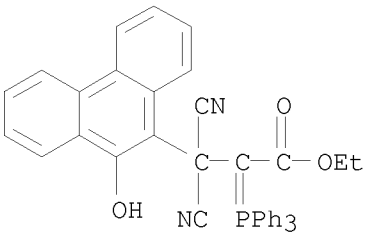
RN 133973-19-0 CAPLUS

CN 9-Phenanthrenepropanoic acid, β,β-dicyano-10-hydroxy-α-(triphenylphosphoranylidene)-, methyl ester (CA INDEX NAME)

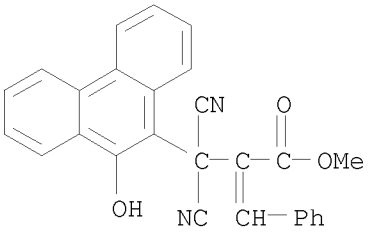


RN 133973-20-3 CAPLUS

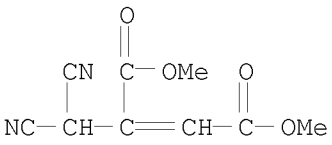
CN 9-Phenanthrenepropanoic acid, β,β-dicyano-10-hydroxy-α-(triphenylphosphoranylidene)-, ethyl ester (CA INDEX NAME)



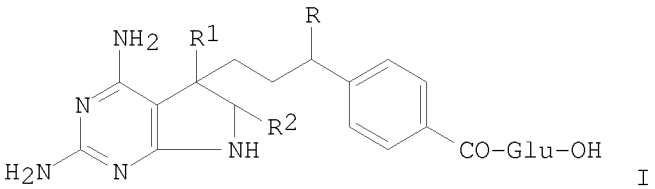
IT 133973-25-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 133973-25-8 CAPLUS
CN 9-Phenanthrenepropanoic acid, β,β-dicyano-10-hydroxy-α-(phenylmethylene)-, methyl ester (CA INDEX NAME)



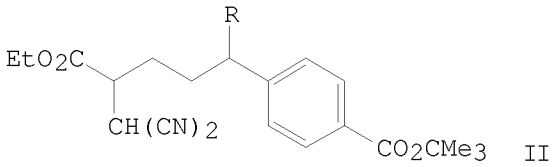
L4 ANSWER 42 OF 68 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1991:121991 CAPLUS
DOCUMENT NUMBER: 114:121991
ORIGINAL REFERENCE NO.: 114:20773a,20776a
TITLE: Reactions of malononitrile with acetylenic esters and ketones [Erratum to document cited in CA113(25):231170y]
AUTHOR(S): Kandeel, Kamal A.; Vernon, John M.; Dransfield, Trevor A.; Fouli, Fouli A.; Youssef, Ahmed S. A.
CORPORATE SOURCE: Dep. Chem., Univ. York, Heslington/York, YO1 5DD, UK
SOURCE: Journal of Chemical Research, Synopses (1990), (12), 406
CODEN: JRPSDC; ISSN: 0308-2342
DOCUMENT TYPE: Journal
LANGUAGE: English
AB An error in the structure for compound 13 has been corrected The error was not reflected in the abstract or the index entries.
IT 130747-61-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of (Erratum))
RN 130747-61-4 CAPLUS
CN 2-Butenedioic acid, 2-(dicyanomethyl)-, dimethyl ester (9CI) (CA INDEX NAME)



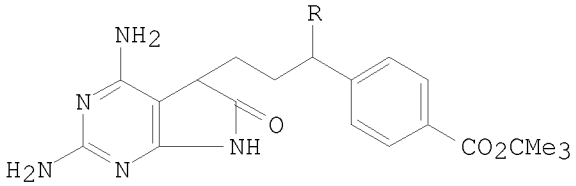
L4 ANSWER 43 OF 68 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1991:82446 CAPLUS
DOCUMENT NUMBER: 114:82446
ORIGINAL REFERENCE NO.: 114:14101a,14104a
TITLE: Novel pyrrolo[2,3-d]pyrimidine antifolates: synthesis and antitumor activities
AUTHOR(S): Miwa, Tetsuo; Hitaka, Takenori; Akimoto, Hiroshi; Nomura, Hiroaki
CORPORATE SOURCE: Res. Dev. Div., Takeda Chem. Ind., Ltd., Osaka, 532, Japan
SOURCE: Journal of Medicinal Chemistry (1991), 34(2), 555-60
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 114:82446
GI



I



II



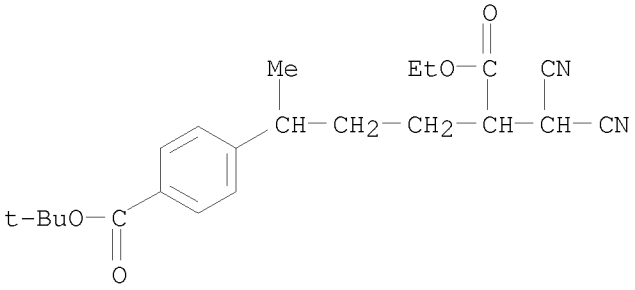
III

AB Title compds. I (R = H, Me; R1 = H, Et; R2R3 = bond, R2 = R3 = H) were prepared as antifolates. A key step was the cyclocondensation of dicyano compound II (R = H, Me) with guanidine-HCl to give pyrrolo[2,3-d]pyrimidines

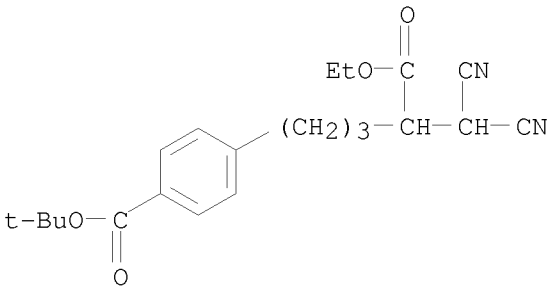
III. III were prepared in several steps from p-RCOC6H4CO2CMe2 and CH3CH:CHCO2Et or BrCH2CH:CHCO2Et. These antifolates were more growth-inhibitory by about 1 order of magnitude than methotrexate (MTX) against KB human epidermoid carcinoma cells and A549 human nonsmall cell lung carcinoma cells in in vitro culture.

IT 125991-47-1P 130351-33-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclocondensation of, with guanidine)

RN 125991-47-1 CAPLUS
CN Benzenepentanoic acid, α-(dicyanomethyl)-4-[(1,1-dimethylethoxy)carbonyl]-δ-methyl-, ethyl ester (CA INDEX NAME)

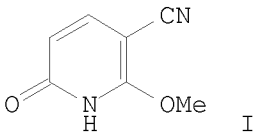


RN 130351-33-6 CAPLUS
CN Benzenepentanoic acid, α-(dicyanomethyl)-4-[(1,1-dimethylethoxy)carbonyl]-, ethyl ester (CA INDEX NAME)



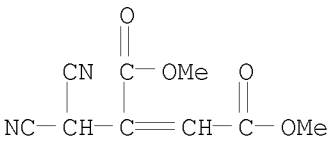
L4 ANSWER 44 OF 68 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1990:631170 CAPLUS
DOCUMENT NUMBER: 113:231170
ORIGINAL REFERENCE NO.: 113:39001a,39004a
TITLE: Reactions of malononitrile with acetylenic esters and ketones
AUTHOR(S): Kandeel, Kamal A.; Vernon, John M.; Dransfield, Trevor A.; Fouli, Fouli A.; Youssef, Ahmed S. A.
CORPORATE SOURCE: Dep. Chem., Univ. York, Heslington/York, YO1 5DD, UK
SOURCE: Journal of Chemical Research, Synopses (1990), (9), 276-7
CODEN: JRPSDC; ISSN: 0308-2342

DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 113:231170
GI

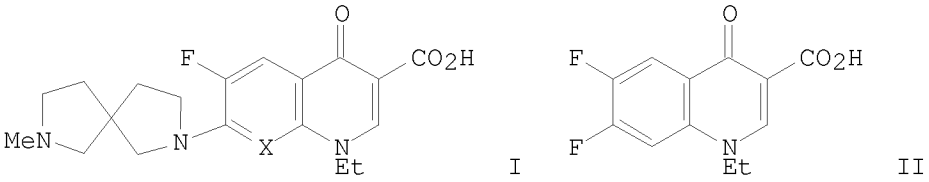


I

AB The addition of malononitrile to acetylenic esters and acetylenic ketones catalyzed by sodium alkoxides gave 3- and 5-cyano-2-pyridones, e.g., I, 2-cyano- and 2,6-dicyanoaniline, and other products.
IT 130747-61-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 130747-61-4 CAPLUS
CN 2-Butenedioic acid, 2-(dicyanomethyl)-, dimethyl ester (9CI) (CA INDEX NAME)



L4 ANSWER 45 OF 68 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1990:497432 CAPLUS
DOCUMENT NUMBER: 113:97432
ORIGINAL REFERENCE NO.: 113:16453a,16456a
TITLE: Quinolone antibacterial agents substituted at the 7-position with spiroamines. Synthesis and structure-activity relationships
AUTHOR(S): Culbertson, Townley P.; Sanchez, Joseph P.; Gambino, Laura; Sesnie, Josephine A.
CORPORATE SOURCE: Parke-Davis Pharm. Res. Div., Warner-Lambert Co., Ann Arbor, MI, 48105, USA
SOURCE: Journal of Medicinal Chemistry (1990), 33(8), 2270-5
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 113:97432
GI



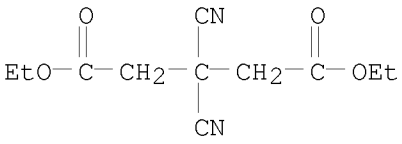
I II

AB Fluoroquinolone antibacterials having the 7-position (10-position of pyridobenzoxazines) substituted with 2,7-diazaspiro[4.4]nonane, 1,7-diazaspiro[4.4]nonane, or 2,8-diazaspiro[5.5]undecane (e.g. I (X = CF, CH, N) were prepared and their biol. activities were compared with piperazine and pyrrolidine substituted analogs. Most exhibited potent Gram-pos. and Gram-neg. activity, especially when side chain was N-alkylated. Thus, the quinolinecarboxylic acid II was treated with 2-methyl-2,7-diazaspiro[4.4]nonane to give I (X = CH).

IT 77415-69-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(reductive cyclization of)

RN 77415-69-1 CAPLUS

CN Pentanedioic acid, 3,3-dicyano-, diethyl ester (9CI) (CA INDEX NAME)



L4 ANSWER 46 OF 68 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1990:235871 CAPLUS

DOCUMENT NUMBER: 112:235871

ORIGINAL REFERENCE NO.: 112:39805a,39806a

TITLE: New gem-dicyanocyclobutane-containing hydroxyesters

AUTHOR(S): Mori, Shojhi; Kakuchi, Toyoji; Padias, Anne Buyle; Hall, H. K., Jr.

CORPORATE SOURCE: Chem. Dep., Univ. Arizona, Tucson, AZ, 85721, USA

SOURCE: Journal of Polymer Science, Part A: Polymer Chemistry (1990), 28(3), 551-8
CODEN: JPACEC; ISSN: 0887-624X

DOCUMENT TYPE: Journal

LANGUAGE: English

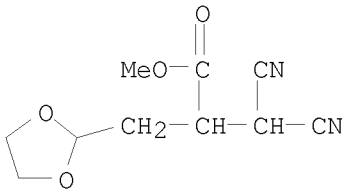
AB Six gem-dicyanocyclobutanes containing carbomethoxy and hydroxyl/acetoxy functions were synthesized by cycloaddn. of the appropriate vinyl ethers or alkoxystyrenes to Me β,β-dicyanoacrylate. They were too thermally liable to allow polycondensation to potentially piezoelec. linear polyesters.

IT 127396-28-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and attempted polymerization of)

RN 127396-28-5 CAPLUS

CN 1,3-Dioxolane-2-propanoic acid, α-(dicyanomethyl)-, methyl ester

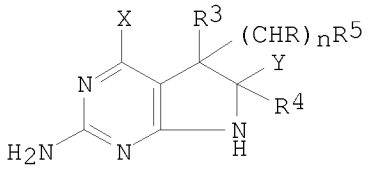
(CA INDEX NAME)



L4 ANSWER 47 OF 68 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1990:158968 CAPLUS
DOCUMENT NUMBER: 112:158968
ORIGINAL REFERENCE NO.: 112:26887a,26890a
TITLE: Preparation of N-[(pyrrolopyrimidinylalkyl)benzoyl]glutamates as neoplasm inhibitors
INVENTOR(S): Akimoto, Hiroshi; Hitaka, Takenori; Miwa, Tetsuo
PATENT ASSIGNEE(S): Takeda Chemical Industries, Ltd., Japan
SOURCE: Eur. Pat. Appl., 24 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 334636	A2	19890927	EP 1989-302851	19890322 <--
EP 334636	A3	19910502		
EP 334636	B1	19961023		
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
NO 8901206	A	19890925	NO 1989-1206	19890320 <--
NO 169490	B	19920323		
NO 169490	C	19920701		
US 4997838	A	19910305	US 1989-326901	19890321 <--
DK 8901437	A	19890925	DK 1989-1437	19890322 <--
DK 173980	B1	20020325		
AT 144513	T	19961115	AT 1989-302851	19890322 <--
ES 2092994	T3	19961216	ES 1989-302851	19890322 <--
CA 1340794	C	19991019	CA 1989-594699	19890323 <--
CN 1037513	A	19891129	CN 1989-101681	19890324 <--
CN 1029970	B	19951011		
HU 51624	A2	19900528	HU 1989-1517	19890324 <--
HU 203105	B	19910528		
JP 02167281	A	19900627	JP 1989-72235	19890324 <--
JP 07005599	B	19950125		
HU 55396	A2	19910528	HU 1990-8458	19890324 <--
HU 215928	B	19990329		
US 5106974	A	19920421	US 1990-578258	19900906 <--
NO 9100661	A	19890925	NO 1991-661	19910219 <--
NO 178304	B	19951120		
NO 178304	C	19960228		
US 5296600	A	19940322	US 1992-824106	19920122 <--

US 5539113 A 19960723 US 1993-161533 19931206 <--
PRIORITY APPLN. INFO.: JP 1988-71149 A 19880324
JP 1988-245379 A 19880929
NO 1989-1206 A1 19890320
US 1989-326901 A3 19890321
US 1990-578258 A3 19900906
US 1992-824106 A3 19920122
OTHER SOURCE(S): CASREACT 112:158968; MARPAT 112:158968
GI



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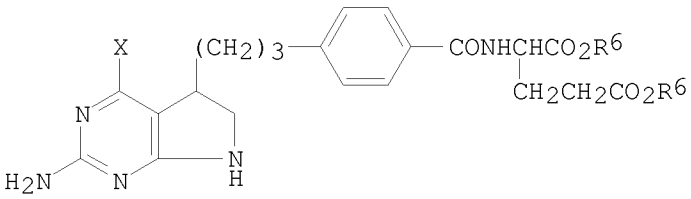


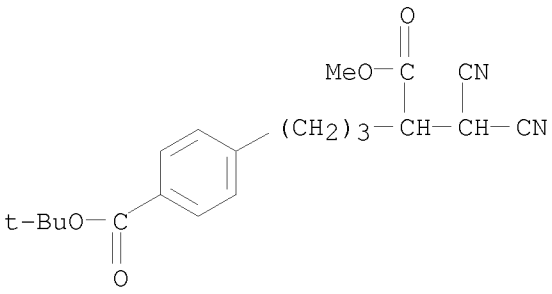
III

AB The title compds. [I; R = H, F, alkyl, alkenyl, alkynyl; R3, R4 = H; R3R4 = bond; R5 = C6H4(CONHCHR1CH2CH2R2)-4; R1,R2 = (un)esterified CO2H; X = NH2, OH; Y = H, NH2, OH; n = 2-4] were prepared Thus, 4-(Me3CO2C)C6H4(CH2)3CH[CH(CN)2]CO2Me (preparation given) was refluxed 28 h with (H2N)2C:NH.HCl in Me3COH containing Me3COK to give I [R = R3 = H, R5 = C6H4(CO2CMe3)-4, X = NH2, n = 3] (II; R4Y = O) which was hydrogenated to II (R4 = Y = H). The latter was hydrolyzed and the product condensed with di-Et L-glutamate to give title compound III (R6 = Et, X = NH2) which was hydrolyzed to III (R6 = H, X = OH) which had IC50 of 0.0006 μg/mL against human nasopharyngeal cancer KB cells in vitro.

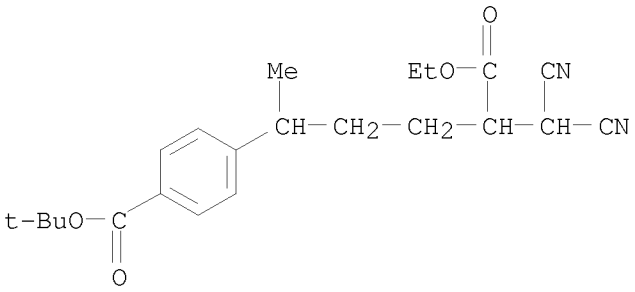
IT 125991-38-0P 125991-47-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, in preparation of neoplasm inhibitors)

RN 125991-38-0 CAPLUS

CN Benzenepentanoic acid, α-(dicyanomethyl)-4-[(1,1-dimethylethoxy)carbonyl]-, methyl ester (CA INDEX NAME)



RN 125991-47-1 CAPLUS
CN Benzenepentanoic acid, α-(dicyanomethyl)-4-[(1,1-dimethylethoxy)carbonyl]-δ-methyl-, ethyl ester (CA INDEX NAME)



L4 ANSWER 48 OF 68 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1989:415389 CAPLUS
DOCUMENT NUMBER: 111:15389
ORIGINAL REFERENCE NO.: 111:2625a,2628a
TITLE: Color photothermographic elements containing leuco compounds
INVENTOR(S): Sakizadeh, Kumars; Weigel, David C.; Grieve, Duncan; Poon, Stephen S. C.; Thien, Tran V.
PATENT ASSIGNEE(S): Minnesota Mining and Manufacturing Co., USA
SOURCE: Eur. Pat. Appl., 35 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 294099	A2	19881207	EP 1988-304771	19880526 <--
EP 294099	A3	19890531		
EP 294099	B1	19930818		
R: BE, DE, FR, GB, IT				
US 4883747	A	19891128	US 1988-200665	19880531 <--
CA 1331107	C	19940802	CA 1988-568396	19880602 <--
AU 8817345	A	19881208	AU 1988-17345	19880603 <--
AU 606162	B2	19910131		

JP 02032332	A	19900202	JP 1988-145566		19880613 <--
JP 2590204	B2	19970312			
US 4923792	A	19900508	US 1989-368566		19890620 <--
PRIORITY APPLN. INFO.:			GB 1987-12961	A	19870603
			US 1988-200665	A1	19880531

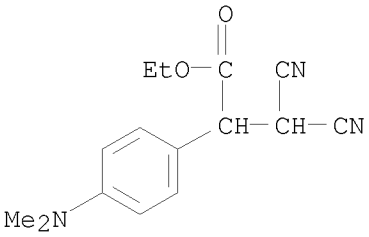
OTHER SOURCE(S): CASREACT 111:15389; MARPAT 111:15389

AB A photothermog. material comprises Ag halide in reactive association with a Ag salt of an organic acid and a color-generating reducing agent which is a leuco compound oxidizable by Ag ions into a colored dye of the formula ArR1C(:C(R5)C(R4):)nCR2R3 [n = 0-2; R1 = H, CN, C1-5 alkyl, aryl, CO2R6; R6 = C1-5 alkyl or aryl; R2, R3 = CN, NO2, CO2R6, SO2R6, COR6; R3 and R2 may combine together to form a ring; R4, R5 = H, CN, C1-5 alkyl, or R4 and R5 together may form a ring; Ar = thienyl, furyl, phenyl]. The material produces images with improved color stability. Thus, a green-yellow image was produced with a photothermog. material incorporating leuco form of (p-dimethylaminobenzylidene)dimethylbarbituric acid.

IT 121246-61-5
RL: USES (Uses)
(photothermog. material containing, for improved image stability)

RN 121246-61-5 CAPLUS

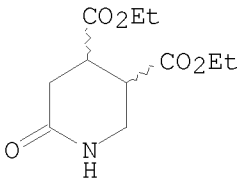
CN Benzeneacetic acid, α-(dicyanomethyl)-4-(dimethylamino)-, ethyl ester (CA INDEX NAME)



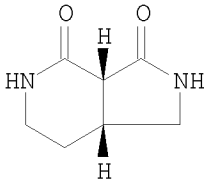
L4 ANSWER 49 OF 68 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER:	1988:570272 CAPLUS
DOCUMENT NUMBER:	109:170272
ORIGINAL REFERENCE NO.:	109:28239a,28242a
TITLE:	Synthesis and cognition-activating properties of some mono- and bicyclic lactam derivatives
AUTHOR(S):	Altomare, Cosimo; Carotti, Angelo; Casini, Giovanni; Cellamare, Saverio; Ferappi, Marcello; Gavuzzo, Enrico; Mazza, Fernando; Pantaleoni, Giancarlo; Giorgi, Raffaele
CORPORATE SOURCE:	Dip. Farm.-Chim., Univ. Bari, Bari, Italy
SOURCE:	Journal of Medicinal Chemistry (1988), 31(11), 2153-8 CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE:	Journal
LANGUAGE:	English
OTHER SOURCE(S):	CASREACT 109:170272

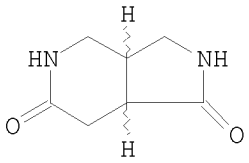
GI



I



II



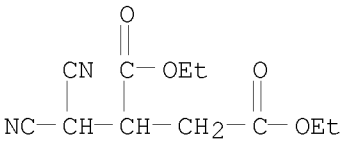
III

AB Upon reductive cyclization cyano esters EtO2CCH2CH(CO2Et)CHRCN (R = CO2Et, cyano) and NCCH2CH(CN)CH(CO2Et)2 yielded piperidones and perhydropyrrolo[3,4-c]pyridine lactams I, II and III, resp. generally as a mixture of diastereomeric cis-trans forms. X-ray crystallog. anal. were carried out on cis-II and III. A series of neuropsychopharmacol. tests performed on I, II, and III indicated that they are generally nontoxic even at high doses (up to 1000 mg/kg i.p.)9. The cognition activating properties of lactams cis- and trans-I, cis-II, and III were evaluated in enhancing retention for passive avoidance learning in rats without and after electroconvulsive shock (ECS); compds. cis-I and III were found to be more potent than piracetam in the amnesia-reversal testing.

IT 82584-86-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(reductive cyclization of, cyclic lactams from)

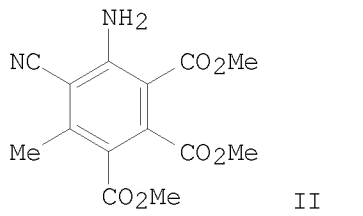
RN 82584-86-9 CAPLUS

CN Butanedioic acid, (dicyanomethyl)-, diethyl ester (9CI) (CA INDEX NAME)



L4 ANSWER 50 OF 68 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1988:94172 CAPLUS
DOCUMENT NUMBER: 108:94172
ORIGINAL REFERENCE NO.: 108:15475a,15478a
TITLE: Addition of ylidenemalononitriles onto dimethyl acetylenedicarboxylate
AUTHOR(S): Gewald, Karl; Hain, Ute; Gruner, Margit
CORPORATE SOURCE: Sekt. Chem., Tech. Univ. Dresden, Dresden, DDR-8027, Ger. Dem. Rep.
SOURCE: Zeitschrift fuer Chemie (1987), 27(1), 32-4
CODEN: ZECEAL; ISSN: 0044-2402
DOCUMENT TYPE: Journal
LANGUAGE: German
OTHER SOURCE(S): CASREACT 108:94172
GI



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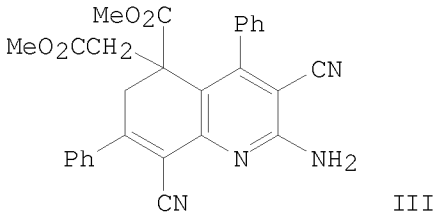
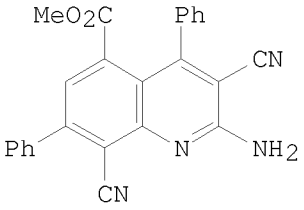
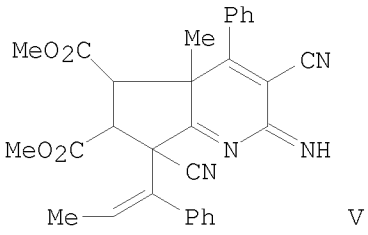


III



IV



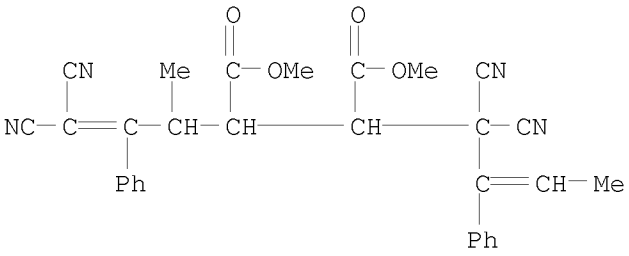
V

AB (NC)2C:CMeCH2CO2Me and MeO2CC.tplbond.CCO2Me (I) in the presence of K2CO3 cycloadded to give 49% aniline II. (NC)2C:CPhMe and I, treated with Et3N, gave 30% dihydroquinoline III, which was aromatized by heating at 270° in Na-MeOH to 80% quinolinecarboxylate IV. (NC)2C:CPhEt and I gave 29% (NC)2C:CPhCHMeCH(CO2Me)CH(CO2Me)C(CN)2CPh:CHMe, which cyclized to cyclopentapyridinedicarboxylate V.

IT 112754-03-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and thermal intramol. cyclization of)

RN 112754-03-7 CAPLUS

CN Butanedioic acid, 2-(3,3-dicyano-1-methyl-2-phenyl-2-propenyl)-3-(1,1-dicyano-2-phenyl-2-butenyl)-, dimethyl ester (9CI) (CA INDEX NAME)



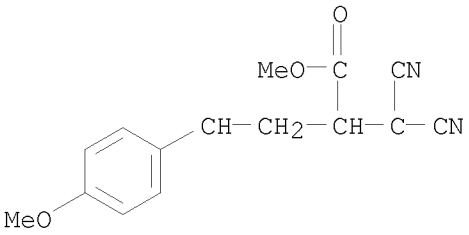
L4 ANSWER 51 OF 68 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1987:597249 CAPLUS
DOCUMENT NUMBER: 107:197249
ORIGINAL REFERENCE NO.: 107:31627a,31630a
TITLE: Influence of the solvent on the nature of a tetramethylene biradical intermediate
AUTHOR(S): Padias, Anne Buyle; Hall, H. K., Jr.
CORPORATE SOURCE: Chem. Dep., Univ. Arizona, Tucson, AZ, 85721, USA
SOURCE: Journal of Organic Chemistry (1987), 52(20),

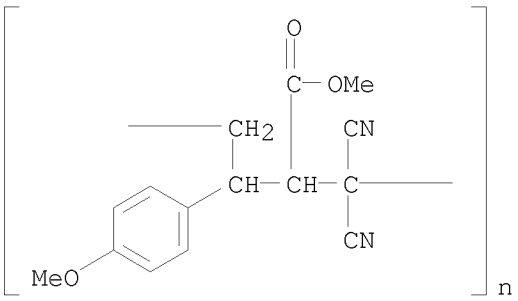
4536-9
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 107:197249

AB In the spontaneous thermal reactions of p-methoxystyrene and Me 3,3-dicyanoacrylate, several reaction products are observed: a 1/1 alternating copolymer, a double Diels-Alder adduct, and the cyclobutane adduct. In dipolar aprotic solvents, no polymerization occurs, and the double Diels-Alder adduct is favored; in protic polar solvents cyclobutane formation competes with copolymn. In nonpolar solvents, copolymn. dominates. A biradical tetramethylene species is proposed as the key intermediate. In polar solvents, this biradical exhibits considerable polar character, and Coulombic attraction between the termini favors the coiled or gauche conformation, leading preferentially to cycloadducts. In nonpolar solvents, the trans conformation initiates the polymerization The main factors influencing the products are the solvent polarity and the ability of the solvent to interact with the biradical.

IT 110193-00-5
RL: PRP (Properties)
(conformation and spin and electron d. of, solvent effects on)
RN 110193-00-5 CAPLUS
CN 1,4-Butanediyl, 1,1-dicyano-2-(methoxycarbonyl)-4-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



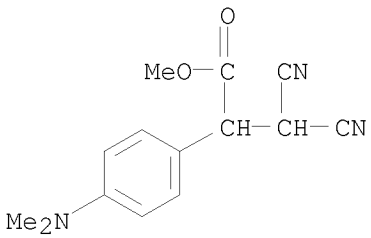
IT 110193-05-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 110193-05-0 CAPLUS
CN Poly[1,1-dicyano-2-(methoxycarbonyl)-3-(4-methoxyphenyl)-1,4-butanediyl] (9CI) (CA INDEX NAME)



L4 ANSWER 52 OF 68 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1987:196834 CAPLUS
DOCUMENT NUMBER: 106:196834
ORIGINAL REFERENCE NO.: 106:31929a,31932a
TITLE: Cationic polymerization of nitrogen-containing electron-rich vinyl monomers by electrophilic olefins and their cyclobutane cycloadducts
AUTHOR(S): Abdelkader, Mohamed; Padias, Anne Buyle; Hall, H. K., Jr.
CORPORATE SOURCE: Chem. Dep., Univ. Arizona, Tucson, AZ, 85721, USA
SOURCE: Macromolecules (1987), 20(5), 944-8
CODEN: MAMOBX; ISSN: 0024-9297
DOCUMENT TYPE: Journal
LANGUAGE: English

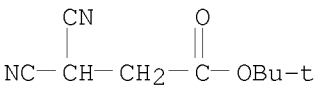
AB The major pathways for the reactions of very electron-rich N-containing olefins with several electrophilic olefins were studied. N-Ethyl-3-vinylcarbazole (I) [1486-07-3], N-vinylcarbazole (II) [1484-13-5], and p-(dimethylamino)styrene (III) [2039-80-7] underwent kinetic cyclobutane formation with an electrophilic olefin without a leaving group, Me β,β-dicyanoacrylate (IV) [82849-50-1], and one with a weak β-leaving group, tetracyanoethylene (V) [670-54-2]. The third electrophilic olefin, β,β-dicyanovinyl chloride (VI) [10472-09-0], had a strong β-leaving group and readily initiated the cationic polymerization of I and II and oligomerization of III. If an excess of donor olefin was used, IV, V, and VI all initiated cationic homopolymn. of I and II, while III only led to oligomers, as it did with conventional Broensted initiators. Cationic initiation by their own cyclobutane adducts was observed for the very electron-rich monomers I and II. Postcyanovinylation of the formed polymers by the electrophilic olefins occurred. Incorporation of a β-leaving group enhanced the initiating ability of the electrophilic olefins and N-carbazyl and N-ethyl-3-carbazyl were overall the most effective donor substituents favoring cationic homopolymn.

IT 107540-79-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, from dimethylaniline and dicyanovinyl compound)
RN 107540-79-4 CAPLUS
CN Benzeneacetic acid, α-(dicyanomethyl)-4-(dimethylamino)-, methyl ester (CA INDEX NAME)

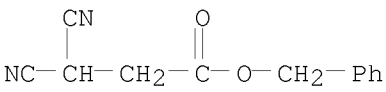


L4 ANSWER 53 OF 68 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1987:33439 CAPLUS

DOCUMENT NUMBER: 106:33439
ORIGINAL REFERENCE NO.: 106:5623a,5626a
TITLE: Synthesis of novel symmetric diamino acids
AUTHOR(S): Reddy, P. Anantha; Erickson, Bruce W.
CORPORATE SOURCE: Rockefeller Univ., New York, NY, 10021, USA
SOURCE: Pept.: Struct. Funct., Proc. Am. Pept. Symp., 9th (1985), 453-6
CODEN: 54ZNAJ
DOCUMENT TYPE: Conference
LANGUAGE: English
AB Sym diamino acids (H2NCH2)2CHCH2CO2H (Aab) 3,5-(H2NCH2X)2C6H3CO2H [X = null, CH2 (Bab)] were prepared from (NC)2CHCH2CO2CMe3 and 3,5-(BrCH2)2C6H3CO2Me. The N,N-bis(tert-butoxycarbonyl) derivative of Aab couples efficiently during solid-phase peptide synthesis. The corresponding derivative of Bab is used in the synthesis of the protein betabellin.
IT 105995-37-7P 105995-39-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrogenation of)
RN 105995-37-7 CAPLUS
CN Propanoic acid, 3,3-dicyano-, 1,1-dimethylethyl ester (CA INDEX NAME)



RN 105995-39-9 CAPLUS
CN Propanoic acid, 3,3-dicyano-, phenylmethyl ester (CA INDEX NAME)



L4 ANSWER 54 OF 68 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1986:496793 CAPLUS
DOCUMENT NUMBER: 105:96793
ORIGINAL REFERENCE NO.: 105:15633a,15636a
TITLE: Zwitterionic tetramethylenes as the common intermediates in the cycloaddition and polymerization reactions of N-vinylcarbazole with electrophilic tetrasubstituted ethylenes: a new explanation for charge-transfer initiation
AUTHOR(S): Gotoh, Tetsuya; Padias, Anne Buyle; Hall, H. K., Jr.
CORPORATE SOURCE: Chem. Dep., Univ. Arizona, Tucson, AZ, 85721, USA
SOURCE: Journal of the American Chemical Society (1986), 108(16), 4920-31
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 105:96793

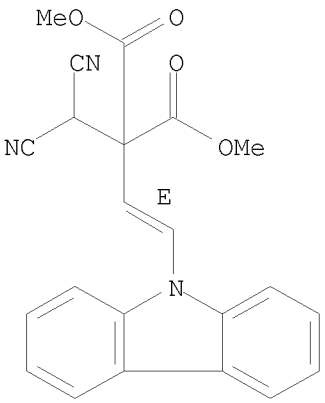
AB The reactions of N-vinylcarbazole (I) with electrophilic tetrasubstituted ethylenes were examples of reactions whose outcomes are manipulated by changes in concentration, structure, and working procedure to form either small mols. (cyclobutanes, 1-butenes) or poly(vinylcarbazole). Equivalent concns. and evaporative workup (organic chemists' conditions) lead to small mols.; a large excess of I and precipitative workup give polymer. The mechanism involves gauche and trans zwitterionic tetramethylenes as intermediates. The former gives cyclobutane reversibly. The latter gives 1-butenes intramol. or adds monomers to form cyclohexanes or eventually polymer. The organic chemical and polymer chemical are unified on this basis. Extensive stereochem. and kinetic support for these propositions is given. Two other proposed mechanisms for these charge-transfer initiations are excluded.

IT 96735-90-9P 102852-12-0P 102852-13-1P
102852-14-2P 102852-38-0P 102852-39-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 96735-90-9 CAPLUS

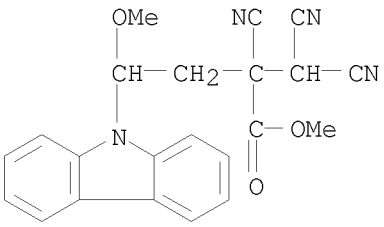
CN Propanedioic acid, [2-(9H-carbazol-9-yl)ethenyl](dicyanomethyl)-, dimethyl ester, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 102852-12-0 CAPLUS

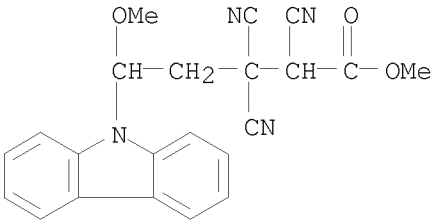
CN 9H-Carbazole-9-butanoic acid, α-cyano-α-(dicyanomethyl)-γ-methoxy-, methyl ester (CA INDEX NAME)



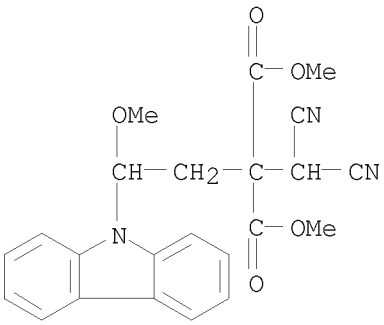
RN 102852-13-1 CAPLUS

CN 9H-Carbazole-9-pentanoic acid, α,β,β-tricyano-δ-

methoxy-, methyl ester (CA INDEX NAME)

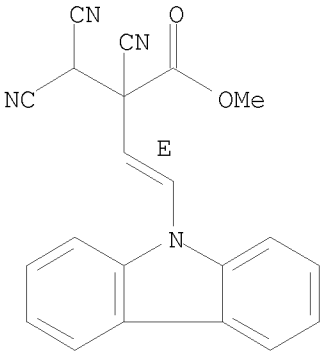


RN 102852-14-2 CAPLUS
CN Propanedioic acid, [2-(9H-carbazol-9-yl)-2-methoxyethyl](dicyanomethyl)-, dimethyl ester (9CI) (CA INDEX NAME)



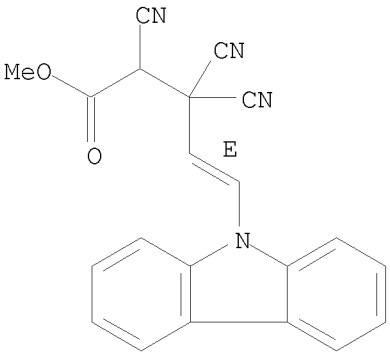
RN 102852-38-0 CAPLUS
CN 3-Butenoic acid, 4-(9H-carbazol-9-yl)-2-cyano-2-(dicyanomethyl)-, methyl ester, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



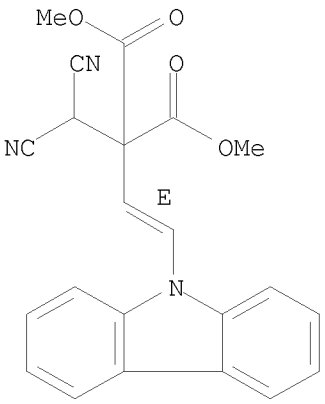
RN 102852-39-1 CAPLUS
CN 4-Pentenoic acid, 5-(9H-carbazol-9-yl)-2,3,3-tricyano-, methyl ester, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

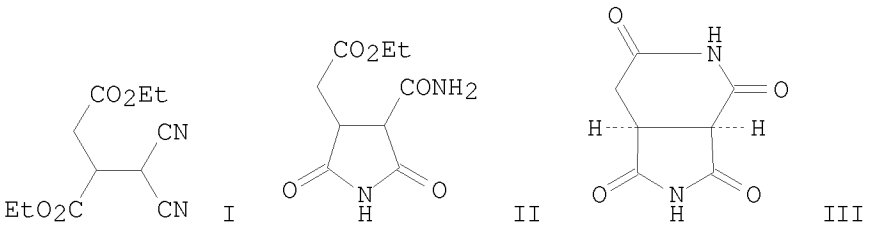


L4 ANSWER 55 OF 68 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1985:406747 CAPLUS
DOCUMENT NUMBER: 103:6747
ORIGINAL REFERENCE NO.: 103:1225a,1228a
TITLE: Zwitterionic tetramethylene intermediates: a new interpretation for "charge-transfer" initiation
AUTHOR(S): Hall, H. K., Jr.; Gotoh, T.
CORPORATE SOURCE: Dep. Chem., Univ. Arizona, Tucson, AZ, 85721, USA
SOURCE: Polymer Preprints (American Chemical Society, Division of Polymer Chemistry) (1985), 26(1), 34-5
CODEN: ACPPAY; ISSN: 0032-3934
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Investigation of the initiation mechanism in polymerization of N-vinylcarbazole (I) [1484-13-5] in the presence of tetracyanoethylene [670-54-2] or di-Me 2,2-dicyanoethylene-1,1-dicarboxylate [82849-49-8] showed that neither the I-cyano compound charge transfer complexes nor the ion-radical pairs formed from them initiated polymerization The initiating species was the gauche or trans tetramethylene zwitterion formed as an intermediate from the charge-transfer complex. This finding indicated that cyclobutanes initiated vinyl polymerization The mechanism and the kinetics of the zwitterionic initiation were discussed.
IT 96735-90-9
RL: CAT (Catalyst use); USES (Uses)
(catalysts, for vinylcarbazole polymerization)
RN 96735-90-9 CAPLUS
CN Propanedioic acid, [2-(9H-carbazol-9-yl)ethenyl](dicyanomethyl)-, dimethyl ester, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

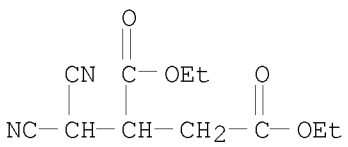


L4 ANSWER 56 OF 68 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1983:488082 CAPLUS
DOCUMENT NUMBER: 99:88082
ORIGINAL REFERENCE NO.: 99:13589a,13592a
TITLE: Tetraoxo derivatives of perhydropyrrolo[3,4-c]pyridine
AUTHOR(S): Ferappi, M.; Carotti, A.; Casini, G.; De Laurentis, N.; Giardina, D.; Cingolani, G. M.; Gavuzzo, E.; Mazza, F.
CORPORATE SOURCE: Ist. Chim. Farm. Tossicol., Univ. Bari, Bari, 70126, Italy
SOURCE: Journal of Heterocyclic Chemistry (1983), 20(2), 439-46
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 99:88082
GI



AB Michael adducts from di-Et furmarate with malonic esters or nitriles were cyclized to succinimide intermediates which, after glutarimide ring closure, afforded several N-Me and N-benzyl derivs. of cis-1,3,4,6-tetraoxoperhydropyrrolo[3,4-c]pyridine whose configuration was demonstrated by x-ray crystal structure anal. Thus, treating the adduct I with H2SO4 gave succinimide II which was treated with NaOEt in EtOH or tosyl acid in xylene to give pyrrolopyridine III.
IT 82584-86-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

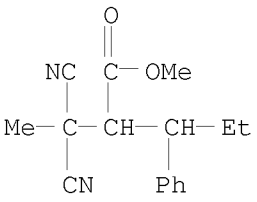
(Reactant or reagent)
(preparation and cyclization of, pyrrolidine from)
RN 82584-86-9 CAPLUS
CN Butanedioic acid, (dicyanomethyl)-, diethyl ester (9CI) (CA INDEX NAME)



L4 ANSWER 57 OF 68 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1982:582893 CAPLUS
DOCUMENT NUMBER: 97:182893
ORIGINAL REFERENCE NO.: 97:30617a,30620a
TITLE: Dimethyl 1,1-dicyanoethene-2,2-dicarboxylate, a new electrophilic olefin
AUTHOR(S): Hall, H. K., Jr.; Sentman, R. C.
CORPORATE SOURCE: Dep. Chem., Univ. Arizona, Tucson, AZ, 85721, USA
SOURCE: Journal of Organic Chemistry (1982), 47(23), 4572-7
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
AB dimethyl 1,1-dicyanoethene-2,2-dicarboxylate (I) [82849-49-8] was synthesized via a Knoevenagel condensation. I spontaneously copolymerizes with electron-rich olefins such as styrene [100-42-5] and p-methylstyrene [622-97-9]. In the copolymn., the bulky growing styryl radicals add to the dicyano-bearing carbon of I. Cyclobutane adducts are obtained in thermal reactions with styrene, p-methylstyrene, p-methoxystyrene [637-69-4], and vinyl ethers via a tetramethylene intermediate. Bond formation occurs at the diester end of I due to the greater stabilization provided by the dicyano group and the minimal steric requirements of the attacking methylene.
IT 82849-58-9P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and NMR spectra of)
RN 82849-58-9 CAPLUS
CN Benzenepropanoic acid, α-(1,1-dicyanoethyl)-β-ethyl-, methyl ester, polymer with ethenylbenzene (9CI) (CA INDEX NAME)

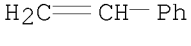
CM 1

CRN 82917-40-6
CMF C16 H18 N2 O2

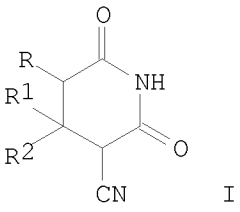


CM 2

CRN 100-42-5
CMF C8 H8



L4 ANSWER 58 OF 68 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1982:472220 CAPLUS
DOCUMENT NUMBER: 97:72220
ORIGINAL REFERENCE NO.: 97:12085a,12088a
TITLE: Contribution to the synthesis of the glutarimides. III
AUTHOR(S): Victory, Pedro; Jover, Jose Maria; Sempere, Julian
CORPORATE SOURCE: Dep. Quim. Org., Inst. Quim. Sarria, Barcelona, Spain
SOURCE: Afinidad (1981), 38(376), 491-5
CODEN: AFINAE; ISSN: 0001-9704
DOCUMENT TYPE: Journal
LANGUAGE: Spanish
OTHER SOURCE(S): CASREACT 97:72220
GI

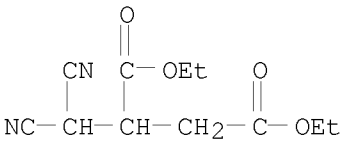


I

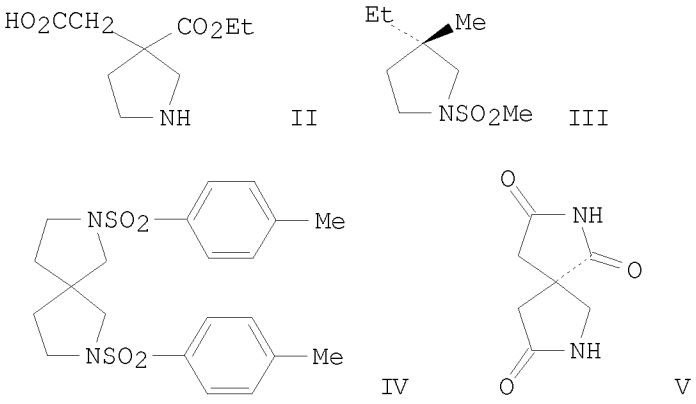
AB Glutarimides I [R = R1 = H, R2 = CO2Et, Ph, 3-furyl, 2-thienyl, Me; R = cyano, R1R2 = (CH2)5; R = Me, R1 = R2 = H] were prepared by treating CH2(CN)2 with R1R2C:CRCO2Et with or without isolation of (NC)2CHCR1R2CHRCO2Et, and acid hydrolysis of the enol ethers. Alternatively R1R2C:CRCO2Et was cyclized with NCCH2CONH2.

IT 82584-86-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and cyclization of)
RN 82584-86-9 CAPLUS
CN Butanedioic acid, (dicyanomethyl)-, diethyl ester (9CI) (CA INDEX NAME)



L4 ANSWER 59 OF 68 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1981:442180 CAPLUS
DOCUMENT NUMBER: 95:42180
ORIGINAL REFERENCE NO.: 95:7221a,7224a
TITLE: Absolute configuration of 2,7-diazaspiro[4,4]nonane. A reassignment
AUTHOR(S): Overberger, C. G.; Wang, David Wei; Hill, Richard K.; Krow, Grant R.; Ladner, David W.
CORPORATE SOURCE: Macromol. Res. Cent., Univ. Michigan, Ann Arbor, MI, 48109, USA
SOURCE: Journal of Organic Chemistry (1981), 46(13), 2757-64
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 95:42180
GI



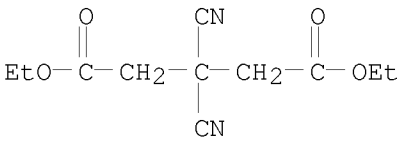
AB The absolute configuration of the axially dissym. spirane 2,7-diazaspiro[4,4]nonane (I), was elucidated as (R)-(-),(S)-(+) in CHCl3 by synthesis of both enantiomers from the centrodissym. intermediate II; the configuration of (R)-(-)-II was correlated with that of (S)-HO2CCMeEtCH2CO2H through the substituted pyrrolidine III. The

configuration thus established for the sulfonamide derivative IV is opposite to that derived earlier (Krow, G. and Hill, R. K., 1968). The source of the original error lies in the preparation of spiroimide V, which is accompanied by almost total racemization when carried out at high temps. A more direct, efficient synthesis of I is described, followed by resolution with dinitrodiphenic acid to give the optically pure enantiomers. Lowe's rule predicts correctly the absolute configurations of several I derivs. but not that of I itself.

IT 77415-69-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and diazaspirononane derivative from)

RN 77415-69-1 CAPLUS

CN Pentanedioic acid, 3,3-dicyano-, diethyl ester (9CI) (CA INDEX NAME)



L4 ANSWER 60 OF 68 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1978:50444 CAPLUS

DOCUMENT NUMBER: 88:50444

ORIGINAL REFERENCE NO.: 88:7949a,7952a

TITLE: The chemistry of 2-oxopropanedinitrile (carbonyl cyanide); XIX. The ene synthesis using 2-oxopropanedinitrile and 1,3-dicarbonyl compounds

AUTHOR(S): Kociolek, K.; Leplawy, M. T.

CORPORATE SOURCE: Inst. Org. Chem., Tech. Univ. Lodz, Lodz, Pol.

SOURCE: Synthesis (1977), (11), 778-80
CODEN: SYNTBF; ISSN: 0039-7881

DOCUMENT TYPE: Journal

LANGUAGE: English

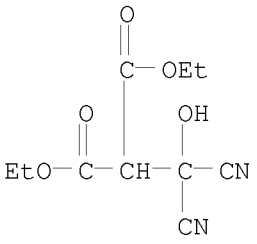
OTHER SOURCE(S): CASREACT 88:50444

AB Reaction of CO(CN)2 with RCOCH2COR1 (I; R = R1 = Ph, 2,4,6-Cl3C6H2, Me; R = Me, F3C, R1 = Ph) in ether at 0° was complete in 1 h and gave RCOCH(COR1)C(CN)2OH (II; R and R1 as before) in 100% yield. Reaction of CO(CN)2 with I (R = R1 = OEt) at room temperature required 20 days and gave II in 43-66% yield.

IT 65305-78-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with aniline)

RN 65305-78-4 CAPLUS

CN Propanedioic acid, (dicyanohydroxymethyl)-, diethyl ester (9CI) (CA INDEX NAME)



L4 ANSWER 61 OF 68 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1973:545978 CAPLUS
DOCUMENT NUMBER: 79:145978
ORIGINAL REFERENCE NO.: 79:23661a,23664a
TITLE: O,O-Dialkylthiophosphoric acid pseudochalcogen acyls
INVENTOR(S): Koehler, Helmut; Gerats, Irmtraut; Eichler, Gerhard; Kochmann, Werner
SOURCE: Ger. (East), 14 pp.
CODEN: GEXXA8
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

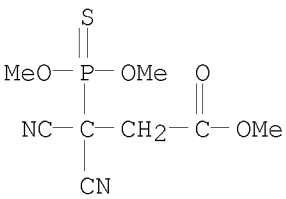
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DD 95374	A1	19730212	DD 1971-156303	19710705 <--

PRIORITY APPLN. INFO.: DD 1971-156303 A1 19710705

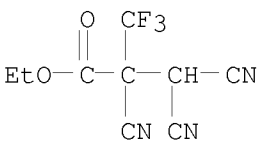
AB (MeO)2P(S)N(CN)CH2CO2R (I) and/or (MeO)2P(:NCN)SCH2CO2R (II) (R = Me or Et), prepared by reacting (MeO)2P(S)NNaCN with XCH2CO2R (X = Br or Cl), gave 95.0, 52.5 and 69.0% mortality for R = Me and 92.5, 51.0 and 55.0% for R = Et at 0.01, 1.0 and 0.05 weight % concentration, resp., against Musca domestica, Sitophylus granarius and Tetranychus urticae, resp. Analogs of I and II wherein the CO2R group was replaced by CONH2 and CONHMe, and (MeO)2P(S)C(CN)2CH2COR and (MeO)2P[: C(CN)2]SCH2COR (R = NHMe or OMe) were also prepared

IT 50605-40-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 50605-40-8 CAPLUS
CN Propanoic acid, 3,3-dicyano-3-(dimethoxyphosphinothioyl)-, methyl ester (CA INDEX NAME)



L4 ANSWER 62 OF 68 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1973:545936 CAPLUS
DOCUMENT NUMBER: 79:145936
ORIGINAL REFERENCE NO.: 79:23657a,23660a
TITLE: Reaction of some fluoroolefins with sodium cyanide
AUTHOR(S): Dyatkin, B. L.; Sterlin, S. R.; Zhuravkova, L. G.; Martynov, B. I.; Knunyants, I. L.
CORPORATE SOURCE: Inst. Elementoorg. Soedin., Moscow, USSR
SOURCE: Zhurnal Organicheskoi Khimii (1973), 9(9), 1786-90
CODEN: ZORKAE; ISSN: 0514-7492
DOCUMENT TYPE: Journal
LANGUAGE: Russian
GI For diagram(s), see printed CA Issue.
AB (CF3)2C:CF2 reacted with 1 equiv of NaCN at -5 to 0° in dioxane containing H2O to give 38% (CF3)2C:CFCN (I), and with excess NaCN in THF containing H2O to give 55% NCC(CF3)2CH(CN)2, a C-H acid of pKa 2.12; analogous treatment of (CF3)2C:CFPh and (CF3)2CHCO2Et yielded 49% NCC(CF3)2CHPhCN and 51% EtO2CC(CN)(CF3)CH(CN)2, resp., after neutralization. Under similar conditions, CF3CF:CF2 afforded 59% CF3[C(CN)2]2Na, although its acid could not be isolated, and (CF3)2C:CFOEt gave 3% (CF3)2C:C(CN)OEt. I reacted with H2SO4 and EtOH to give 25% (CF3)2C:CFCO2Et, with HCl in EtOH to give 20% HOC(CF3)2CHFCONH2, with Et2NH to give 43% (CF3)2C:C(CN)NEt2, with PhNH2 to give 60% (CF3)2CHC(CN):NPh, and with concentrated H2SO4 to give 84% iminolactone (II; R = H), which was converted to its Hg salt (II; R = 1/2 Hg) with HgO in refluxing aqueous Me2CO.
IT 50616-04-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 50616-04-1 CAPLUS
CN Propanoic acid, 2-cyano-2-(dicyanomethyl)-3,3,3-trifluoro-, ethyl ester (CA INDEX NAME)



L4 ANSWER 63 OF 68 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1965:462918 CAPLUS
DOCUMENT NUMBER: 63:62918
ORIGINAL REFERENCE NO.: 63:11492h
TITLE: Reaction of acetylenic esters with cyanoacetic ester and pyridine
AUTHOR(S): Bamfield, P.; Crabtree, A.; Johnson, A. W.
CORPORATE SOURCE: Univ. Nottingham, UK
SOURCE: Journal of the Chemical Society (1965) 4355-62
CODEN: JCSOA9; ISSN: 0368-1769
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Modified structures are suggested for the yellow and the blue adducts from

dimethyl acetylenedicarboxylate, Et cyanoacetate, and pyridine, which were originally prepared and formulated by Diels. The reaction of Me phenylpropiolate, Et cyanoacetate, and pyridine leads to a 1:1:1-adduct in which the pyridine has suffered ring-fission. Various reactions of the adducts are discussed.

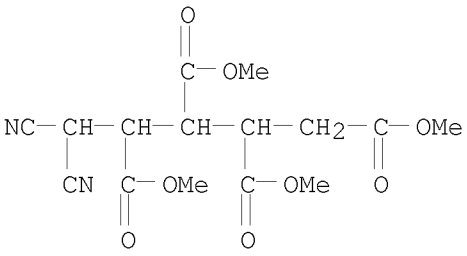
IT 1289-25-4
(Derived from data in the 7th Collective Formula Index (1962-1966))

RN 1289-25-4 CAPLUS

CN 1,2,3,4-Pentanetetracarboxylic acid, 5,5-dicyano-, tetramethyl ester, compd. with pyridine (1:1) (8CI) (CA INDEX NAME)

CM 1

CRN 45287-28-3
CMF C15 H18 N2 O8



CM 2

CRN 110-86-1
CMF C5 H5 N

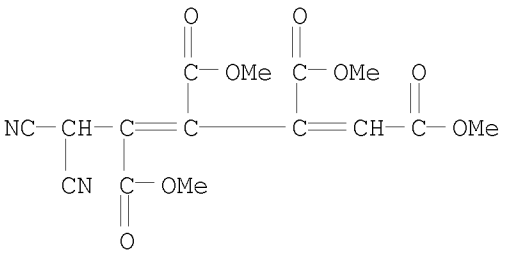
IT 100150-98-9P, Pentadiene-1,2,3,4-tetracarboxylic acid, 5,5-dicyano-, tetramethyl ester, compound with pyridine (1:1)
RL: PREP (Preparation)
(preparation of)

RN 100150-98-9 CAPLUS

CN Pentadiene-1,2,3,4-tetracarboxylic acid, 5,5-dicyano-, tetramethyl ester, compd, with pyridine (7CI) (CA INDEX NAME)

CM 1

CRN 100150-97-8
CMF C15 H14 N2 O8



CM 2

CRN 110-86-1
CMF C5 H5 N

L4 ANSWER 64 OF 68 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1964:484793 CAPLUS
DOCUMENT NUMBER: 61:84793
ORIGINAL REFERENCE NO.: 61:14826g-h,14827a-c
TITLE: 1-Halo-1,2,3,3-tetra(negatively substituted)propanes and their salts
INVENTOR(S): Martin, Elmore L.
PATENT ASSIGNEE(S): E. I. du Pont de Nemours & Co.
SOURCE: 6 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3133084		19640512	US	19600624 <--

PRIORITY APPLN. INFO.: US 19600624

AB Compds. of the general formula [XC(Z):C(Y)C(A)R]- M+ (I), where A, R, Y, Z are electron withdrawing groups such as CN, CO2Et, Bz, or SO2Ph, X is Cl or F, and M is H, Na, K, or a substituted ammonium ion, are dyes for natural and synthetic fibers. Thus, H2C(CN)2 79 in tetrahydrofuran (II) 220 was added with stirring to a dispersion 52 of 51.2% NaH in mineral oil and II 660 at 5-10° during 15 min., the mixture stirred 30 min., then dichlorofumaronitrile 44 in II 220 added during 15 min., II vaccum-distilled at 35-40°, the residual yellow solid dissolved in H2O 250, the pH adjusted to 8 with CO2, then Et4NBr 100 in H2O 200 parts added slowly with stirring, the mixture cooled to 5°, and the yellow crystals of I (A = R = Y = X = CN, Z = Cl, M = Et4N) (III) filtered, washed with 1% Et4NBr, and then H2O. The cake was dissolved in H2O 3500 at 100°, decolorizing carbon 10 added, the solution clarified, cooled to 5°, the long yellow needles filtered, washed with H2O and air-dried, giving 70

parts III, m. 129-31°, λmaximum 387 mμ, ε = 18,200
(MeOH) yellow on cellulose acetate and nylon, brownish yellow on wool and silk. Similarly, other I were prepared as tabulated below: X, Z, Y, A, R, M, % yield, m.p., color, λ (mμ)maximum, ε; Cl, PhN(CO-)2, CN, CN, Me4N, 31 230-5° (decompose), orange, 468, 12,200; Cl, CO2Me, CO2Me, CN, CN, Et4N, 82, 88-90°, yellow, 335, 29,400; Cl, CN, CN, CO2Et, CO2Et, H, 100, b1, 115-20°, yellow (Na salt), -, -; Cl, Bz, Bz, CN, CN, Me4N, 39, 210-12° (decompose), yellow, 416, 27,000; F, CF3, CF3, CN, CN, Pr4N, 81, 84-6°, yellow, -, -; Cl, CN, CN, CN, CN, Me4N, -, 217-18° (decompose), yellow, 386, 17,600; Cl, CN, CN, CN, CN, Pr4N, -, 74-6° (decompose), yellow, 386, 18,100; Cl, CN, CN, CN, CN, Et3NH, -, 63-5° (decompose), yellow, 387, 17,200; Cl, CN, CN, CN, CO2Et, Et4N, 56, 70-2°, yellow, 400, 15,700; Cl, CN, CN, CN, SO2C6H4Me-4, Me4N, 73, 124-6° (decompose), yellow, 387, 17,000; Cl, CN, CN, CN, Bz, Me4N, -, 159-61°, yellow, 414, 17,100; Cl, CN, CN, CN, Bz, Et4N, 30 118-19°, yellow, 420, 16,200; Cl, CN, CN, CN, CN, Pr4N, -, 109-10°, yellow, 412, 17,600; Cl, CF3, CF3, CN, CN, Et4N, 64, 84-5°, yellow, -, -; F, -CF2CF2-, CN, CN, Na, -, -, orange, -, -; Cl, CN, CN, Bz, Bz, Me4n, -, 167°9°, yellow, 422, 8000; Cl, CN, CN, CN, CONHPh, K, -, -, red, -, -; Cl, CN, CN, SO2Ph, SO2Ph, Me4N, -, -, yellow, -, -; Cl, CN, CN, Bz, CO2Et, H, 20, 97-8°, colorless, -, -; Cl, CN, CN, Bz, CO,2Et, Na, yellow;

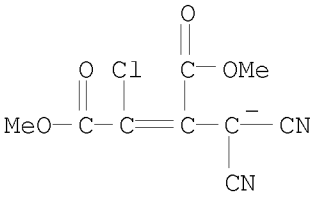
IT 98469-37-5P, Ammonium, tetraethyl, 1,2-dicarboxy-1-chloro-3,3-dicyanopropenide, dimethyl ester
RL: PREP (Preparation)
(preparation of)

RN 98469-37-5 CAPLUS

CN Tetraethylammonium 1,2-dicarboxy-1-chloro-3,3-dicyanopropenide, dimethyl ester (7CI) (CA INDEX NAME)

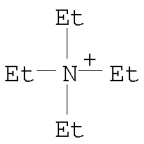
CM 1

CRN 98469-36-4
CMF C9 H6 Cl N2 O4



CM 2

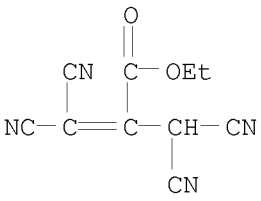
CRN 66-40-0
CMF C8 H20 N



L4 ANSWER 65 OF 68 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1962:429396 CAPLUS
DOCUMENT NUMBER: 57:29396
ORIGINAL REFERENCE NO.: 57:5809h-i,5810c
TITLE: Nitration of cyclohexanecarboxylic acid to caprolactam
AUTHOR(S): Bigot, J. A.; Meijerink, Th. A. J.; Revallier, L. J.
CORPORATE SOURCE: Central Lab., Staatsmijnen, Geleen, Neth.
SOURCE: Recueil des Travaux Chimiques des Pays-Bas (1962), 81, 363-4
CODEN: RTCPA3; ISSN: 0165-0513
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Cyclohexanecarboxylic acid (I) with nitryl hydropyrosulfate in oleum did not give the expected nitrocyclohexane, but 70% caprolactam (II) and a mixture of m-dinitrobenzene and nitrobenzene (total yield 22%, based on I). The mechanism of the reaction is unknown, but there is some evidence that removal of H2O from a nitro derivative is 1 of the steps involved. 1-Methyl-1-nitrocyclohexane with oleum gave a compound, C7H11NO (b2 79°, m. 48°), probably 1-methyl-1-nitrocyclohexene (or its rimer), a compound that could be isolated as such, since it could neither dehydrogenate to a C6H6 derivative, nor disproportionate and subsequently rearrange to II.
IT 94211-18-4P, Acrylic acid, 3,3-dicyano-2-(dicyanomethyl)-, ethyl ester, compound with quinoline 94467-89-7P, Acrylic acid, 3,3-dicyano-2-(dicyanomethyl)-, ethyl ester, compound with NH3
RL: PREP (Preparation)
(preparation of)
RN 94211-18-4 CAPLUS
CN Acrylic acid, 3,3-dicyano-2-(dicyanomethyl)-, ethyl ester, compd. with quinoline (7CI) (CA INDEX NAME)

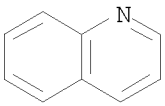
CM 1

CRN 94211-17-3
CMF C10 H6 N4 O2

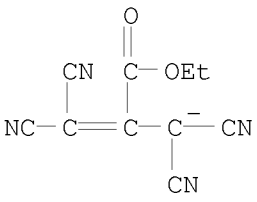


CM 2

CRN 91-22-5
CMF C9 H7 N



RN 94467-89-7 CAPLUS
CN 2-Propenoic acid, 3,3-dicyano-2-(dicyanomethyl)-, ethyl ester, ion(1-), ammonium (9CI) (CA INDEX NAME)



L4 ANSWER 66 OF 68 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1962:429395 CAPLUS
DOCUMENT NUMBER: 57:29395
ORIGINAL REFERENCE NO.: 57:5809e-h
TITLE: Base-catalyzed ring opening of diethyl 1,1,2,2-tetracyanocyclopropane-3,3-dicarboxylate
AUTHOR(S): Regan, T. H.
CORPORATE SOURCE: E. I. du Pont de Nemours & Co., Wilmington, DE
SOURCE: Journal of Organic Chemistry (1962), 27, 2236-7
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB An example of a cyclopropane ring cleavage under very mild conditions was reported. CH2(CN)2 (6.6 g.) in 17.4 g. di-Et oxomalonate was left 3 hrs. with one drop of base catalyst; the solid was collected and shown to be di-Et dihydroxymalonate. Fractionation of the yellow oil gave 11.7 g. di-Et 1,1-dicyanoethylene-2,2-dicarboxylate, b1 86°, n24D 1.4628. An equimolar mixture of this compound and anthracene after heating at 150° gave crystalline product, m. 153.6-5.2° (alc.-H2O). The product resulting from 38 g. CH2(CN)2 and 100 g. di-Et oxomalonate in 250 ml. alc. treated in the cold with 52 g. Br, the solution poured onto 1 kg. ice, and the oil crystallized when left overnight gave 71.5 g. di-Et 1,1,2,2-tetracyanocyclopropane-3,3-dicarboxylate (I), m. 129.6-31.2° (alc.-H2O). I (15 g.) was suspended in 500 ml. Et2O, treated with 15 g. dry NH3, stirred overnight and the mixture filtered to

give 11.4 g. solid, m. 192-201° (decomposition). The filtrate evaporated and the residue stirred with CHCl3 gave 0.5 g. yellow powder, m. 203° (decomposition). The CHCl3 solution evaporated gave Et carbamate, m. 46.6-8.6°. The yellow powder was ammonium 1,1,3,3-tetracyano-2-carbethoxypropenide (II). II in H2O treated with a concentrated aqueous solution of quinolinium chloride gave quinolinium 1,1,3,3-tetracyano-2-carbethoxypropenide, m. 111.5-12.5°. Recrystn. from H2O gave a hydrate, m. 51-2°.

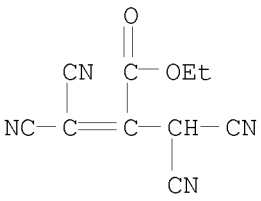
IT 94211-18-4P, Quinoline, compound with Et 3,3-dicyano-2-(dicyanomethyl)-acrylate 94467-89-7P, Acrylic acid, 3,3-dicyano-2-(dicyanomethyl)-, ethyl ester, compound with NH3
RL: PREP (Preparation)
(preparation of)

RN 94211-18-4 CAPLUS

CN Acrylic acid, 3,3-dicyano-2-(dicyanomethyl)-, ethyl ester, compd. with quinoline (7CI) (CA INDEX NAME)

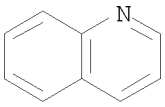
CM 1

CRN 94211-17-3
CMF C10 H6 N4 O2



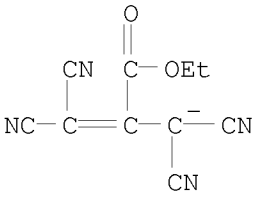
CM 2

CRN 91-22-5
CMF C9 H7 N



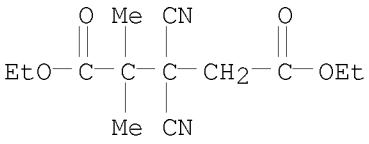
RN 94467-89-7 CAPLUS

CN 2-Propenoic acid, 3,3-dicyano-2-(dicyanomethyl)-, ethyl ester, ion(1-), ammonium (9CI) (CA INDEX NAME)



L4 ANSWER 67 OF 68 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1940:18276 CAPLUS
DOCUMENT NUMBER: 34:18276
ORIGINAL REFERENCE NO.: 34:2801g-i,2802a-b
TITLE: Synthesis of α,α-dimethyltricarballylic and 1-carboxy-cyclopentane-1-α-succinic and 1-carboxy-3-methylcyclopentane-1-α-succinic acids
AUTHOR(S): Desai, R. D.; Sahariya, G. S.
SOURCE: Journal of the University of Bombay, Science: Physical Sciences, Mathematics, Biological Sciences and Medicine (1939), 8(Pt. 3), 235-8
CODEN: JUBSAS; ISSN: 0368-4644
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB When in RR'C(CN)C(CN)CO2Et, R and R' together are cyclopentane or methylcyclopentane rings, there are obtained with CH2BrCO2Et (I) excellent yields of tricarballylic acids which are characterized by their toluidide N-tolylimides. A mixture of the Et sodiocyanoacetate (II) from 24 g. cyanoacetate and 21 g. cyclopentanone cyanohydrin is allowed to stand for 48 h. After addition of 32 g. I the mixture is kept at room temperature for 2 days and then refluxed until it is neutral. The EtOH is distilled off, the residue diluted with H2O and the oil extracted with ether, dried and distilled into 3 fractions, b4 90-120°, 120-65° and 185-7°. The 2nd fraction is retreated with I. Et 1-cyanocyclopentane-1-α-cyanosuccinate (III), b4 185-7°, is obtained in 45% yield. Hydrolysis of III with concentrated H2SO4 gives 1-carboxycyclopentanesuccinic acid (IV), m. 165° (cf. Chatterji, C. A. 31, 7409.7, found 159°). Its anilide N-phenylimide, prepared by heating IV with PhNH2 at 170-5° for 3 h., m. 156°; p-toluidide N-p-tolylimide m. 189-90°. Et 1-cyano-3-methylcyclopentane-1-α-cyanosuccinate (V), prepared as II, b12 205°. Hydrolysis of V gives 1-carboxy-3-methylcyclopentanesuccinic acid, m. 144°; its p-toluidide N-tolylimide m. 167°. Di-Et 2-methyl-3,3-dicyanobutane-3,4-dicarboxylate (VI), prepared from II, Me2C(OH)CN and I, in 45% yield, b5 176-8°. Saponification of VI with H2SO4 gives α,α-dimethyltricarballylic acid, m. 160° (C. found 156°). Its anilide N-phenylimide m. 140°; the p-toluidide N-p-tolylimide m. 170°.
IT 858794-64-6P, Glutaric acid, β,β-dicyano-α,α-

dimethyl-, diethyl ester
RL: PREP (Preparation)
(preparation of)
RN 858794-64-6 CAPLUS
CN Pentanedioic acid, 3,3-dicyano-2,2-dimethyl-, 1,5-diethyl ester (CA INDEX NAME)



L4 ANSWER 68 OF 68 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1938:911 CAPLUS
DOCUMENT NUMBER: 32:911
ORIGINAL REFERENCE NO.: 32:156d-i,157a-i,158a-e
TITLE: 2,3,-Dioxopyrrolines, mononuclear substances related to isatin
AUTHOR(S): Mumm, Otto; Hornhardt, Hans
SOURCE: Berichte der Deutschen Chemischen Gesellschaft [Abteilung] B: Abhandlungen (1937), 70B, 1930-47
CODEN: BDCBAD; ISSN: 0365-9488
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB 5-Phenyl-2,3-dioxopyrroline (I) (C. A. 5, 703) is so extraordinarily similar in appearance and chemical properties to isatin that it may be considered as a mononuclear isatin, and it was hoped that by means of this very reactive substance light might be obtained on some of the controversial questions on isatin, especially the structure of its salts and derivs. The earlier work on I was accordingly resumed and attention was directed to the preparation of analogs of I containing an aliphatic residue instead of
Ph. In order not to weaken the ring unnecessarily, a residue (hexyl) of rather high mol. weight was chosen. As a tertiary residue might also favor the stability of the ring, Me3C was selected for a 2nd series of expts. It was intended to prepare the new compds. by the earlier method. Pinacolone and C6H13COMe were condensed with HCO2R to the hydroxymethylene compds. which with NH2OH yielded the oxazoles through the intermediate oximes. The conversion of the oxazoles into the open-chain methylimide nitriles proceeded as expected and the formation from the nitriles of the desired pyrrolines with alc. HCl undoubtedly occurred, as evidenced by the appearance of the characteristic dark red color, but the products did not crystallize. The planned investigation was therefore continued with aromatic derivs., using p-tolyl instead of Ph compds. These tolyl compds., having higher m. ps., were considerably more stable and crystallized better. The starting point was α-p-tolylisoxazole (II). That the nitrile obtained from II was really p-toluylpyruvonitrile methylimide, RC(OH):CHC(:NMe)CN(R = p-MeC6H4) (III), was shown by the reaction with MeMgI, which gave the normal product, RC(OH)MeCH2C(:NMe)C(:NMgI) (IV), and also the compound RC(NH2)MeCH2C(:NMe)C(:NMgI)Me(V) when the Grignard compound was decomposed with NH4Cl instead of water. RC(OH)MeCH2C(:NMe)C(OH)(NHMgI)M

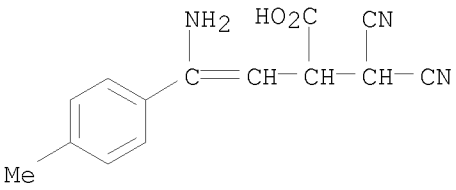
e (VI) was also formed by addition of H2O to IV under the influence of glacial AcOH. III merely treated in the cold with HCl in absolute alc. gave the blood-red di-HCl salt of 5-p-tolyl-2-oxo-3-methyliminopyrroline (VII). The previously assumed intermediate imido ester, RC(OH):CHC(:NMe)C(:NH)OEt (VIII), corresponding to the nitrile, was isolated as its white HCl salt, which readily changes, even in the absence of air, into the dark red derivative of VII. The distribution of the double bonds shown in III probably occurs only under the influence of the HCl, the free nitrile having the tautomeric structure RCOCH:C(NHMe)CN. The outstanding property of the dark red VII.2HCl is the ease with which the NMe group is replaced by O to form the brick-red 5-p-tolyl-2,3-dioxopyrroline (IX). As with isatin, NaOH cleaves the ring in IX to give α-oxo-γ-imino-γ-p-tolylbutyric acid (X) through an intermediate intensely blue alkali salt. Attempts to liberate VII from its HCl salt were unsuccessful. Dilute aqueous alkali or NaHCO3 gave, instead, the yellow-green pseudo base (XI), while excess of concentrated KOH yielded a dark red K salt, C12H11ON2K.2H2O, which regenerated XI with water. NH3 in alc. replaces both the NMe group and the carbonyl O by NH and at the same time 1 mol. alc. is taken up with formation of a product, RC:CH.C(NH2)(OEt).C(:NH).NH (XII), similar in structure to XI; the dark red color immediately produced by HCl shows the ring has not been cleaved. PhNH2 in alc. yields brick-red needles of the 3-phenylimino analog (XIII) of VII. With KOH and also with HCl, XIII forms salts which are red-violet in solution and almost black in the solid state. The HCl salt quant. splits off the HCl at high temps. in vacuo without changing to the brick-red of the free XIII, showing that the salt formation is accompanied by a simultaneous intramol. rearrangement. In water the HCl salt, like that of VII, is hydrolyzed to IX, but attempts to prepare the pseudo base were unsuccessful; instead was obtained XIII into which the K salt also changes on mere exposure to moist air. This difference in behavior and the very different colors show that the salts of VII and XIII have different structures. As with water and PhNH2, the dark red salt of VII also reacts with compds. having a reactive methylene group. Especially smooth, and under the mildest conditions, is the reaction with CH2(CN)2 to give 5-p-tolyl-2-oxo-3-dicyanomethylenepyrroline (XIV), also obtained from IX or XIII. Surprisingly, XIV forms beautiful violet-black needles and dissolves, although difficultly, in alc. with red-violet color, whereas the corresponding isatin derivative is yellow-red, indicating a fundamental difference in structure. When the alc. solution of XIV is treated with a strong base, it immediately turns steel-blue, but, as with the salts of IX, the blue color quickly disappears and the ring is opened; acids precipitate the yellow cleavage product, RC(NH2):CHC[:C(CN)2]CO2H, m. 276°, probably in the form of the inner salt, which with boiling alc. HCl changes through the intermediate RC(NH2):CHC(CO2H):C(CO2H)C(:NH)OEt into the compound RC(NH2):CHC(CO2H):CHC(:NH)OEt (XV). X gently heated with dilute acids yields the dioxo acid. The ring in IX is also cleaved by piperidine, MeNH2 and NH3 to form compds. of the type RC(:NH)CH2COCONC5H11 (XVI). PhNH2 and CH2(CN)2, on the other hand, react with the 3-CO group, leaving the ring intact. The similarity of the dioxopyrrolines to isatin is also shown in their catalytic hydrogenation. There is first formed a light gray, alc.-insol. product (XVII) corresponding to isatyde which in the air rapidly regenerates the original compound If the hydrogenation is continued, the XVII redissolves, and cautious addition of water to the colorless alc. solution ppts. a completely air-stable crystalline product, RC(NH2):CHCH(OH)CO2H (XVIII). Reduction of XIII in alc. proceeds 1 step further, with addition of 2 mols. H and 1 mol. alc. to give the compound

RCH(NH2)CH2CH(NHPh)CO2Et (XIX). For the bearing of the above facts, especially the color phenomena, on the structures of the mononuclear isatins and their derivs., the original should be consulted. Hydroxymethylenepinacolone dioxime (54% yield), m. 84°. α-tert-Butylisoxazole, b760 156°; its methosulfate with KCN in water at 0° gave 82% trimethylacetopyruvonitrile methylimide, m. 42°, hydrolyzed by cold concentrated HCl to the pyruvic acid, crystals with 1 H2O, m. 64°, and by dilute HCl to the amide, m. 115°; in cold absolute alc. with HCl gas the nitrile imide gave a dark red oil which with 2 N NaOH or 50% AcOH yielded α-oxo-α-imino-δ,δ-dimethylcaproic acid, m. 185° (gas evolution). When the red oil was carefully freed from adhering HCl, simple solution in ordinary alc. resulted in ring cleavage (probably by the water in the alc.), but AcOEt precipitated a crystalline substance, m. 186°, insol. in all solvents except alc. and water, which on gentle warming with water gave trimethylacetopyruvic acid methylimide, m. 183°. Hydroxymethylenemethyl hexyl ketone oxime, m. 118°. α-Hexylisoxazole, b11 97-8°, was analyzed as the chloroplatinate, C20H36O2N2PtCl6, obtained from the methosulfate with PtCl4. α,α-Dioxodecanonitrile α-methylimide, oil decomposing on distillation, even in a high vacuum; α,α-dioxodecanamide, m. 99°. Hydroxymethylene-p-methylacetophenone oxime (67% yield), m. 133°. II, m. 60°. III, light yellow, m. 126°. IV (3 g. from 2 g. II and 2.2 mol. MeMgI boiled 2 h. in ether), yellow, m. 175° (decomposition); heated a short time or allowed to stand 1 day at room temperature in glacial AcOH, it changed into VI, rhombic tables, red-brown in incident light, m. 183° (decomposition). V, m. 197°, soluble in AcOH with wine-red color, easily soluble in dilute HCl and repptd. by NaOH. VII.2HCl (78%), sinters and carbonizes at 183°; picrate, intensely red, m. 192°. VIII.HCl, from III in cold dioxane with 0.662 N HCl in absolute alc., decomps. 145°. If in the treatment of III with alc.-HCl water is present even only in traces the reaction proceeds in part in an entirely different way, giving in addition to the dark red salt Me p-toluylpyruvate, m. 84°; free acid, crystals with 1 H2O, m. 143°. Ag salt of VII, red needles with 1 MeOH, decomposing 172°. Cu salt, (C12H11ON2)2Cu.4H2O, green, m. 191° (decomposition). XII, m. 153°. IX, precipitated quant. in about 6 h. from VII.2HCl in 20 parts cold water, m. 229-30°; a cold alc. suspension treated with somewhat less than 1 mol. EtOK-solution at once becomes blue-violet and soon deposits the K salt, C11H8O2NK.2H2O, which is not very stable even when dry; one sample had become yellowish after 14 days. Alc. IX treated with aqueous NaOH also immediately turns blue-violet but the color rapidly disappears and on cautious acidification X, m. 155°, seps. Piperidide (XVI), m. 184°. Amide, C11H12O2N2.0.5H2O, m. 179°. Methylamide (0.5H2O), m. 169°. XVIII, turns brown and carbonizes 245-50°. XIII, m. 237°. XIX, m. 123°. XIV was obtained in 92% yield; its melting or decomposition point is so extraordinarily high that it could not be determined XV.2HCl, lemon-yellow, m. 148-9°.

IT 855234-21-8P, 3-Butenoic acid, 4-amino-2-(dicyanomethylene)-4-p-tolyl-
RL: PREP (Preparation)
(preparation of)

RN 855234-21-8 CAPLUS

CN 3-Butenoic acid, 4-amino-2-(dicyanomethyl)-4-(4-methylphenyl)- (CA INDEX NAME)


NH2
HO2C
CN
C
CH
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